

chain nodes :
6 7 8 10 11
ring nodes :
1 2 3 4 5
chain bonds :
1-10 6-7 6-8 7-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11

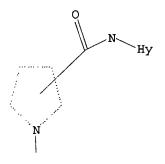
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom
Generic attributes:
11:
Number of Carbon Atoms: less than 7

Number of Hetero Atoms : less than 2
Type of Ring System : Monocyclic

Element Count : Node 11: Limited C,C4 S,S1

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 11:59:12 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 87815 TO ITERATE

2.3% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 1738707 TO 1773893

PROJECTED ANSWERS: 0 TO

L2 0 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 11:59:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 753988 TO ITERATE

41.1% PROCESSED 720923 ITERATIONS 310 ANSWERS

51.4% PROCESSED 902313 ITERATIONS 316 ANSWERS

55.8% PROCESSED 978997 ITERATIONS 316 ANSWERS

57.0% PROCESSED 1000000 ITERATIONS 316 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.52

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

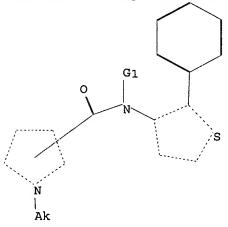
PROJECTED ITERATIONS: 1753988 TO 1753988

PROJECTED ANSWERS: 484 TO 624

L3 316 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10680346B.str



20 21 22 19 23 16 18 8 7 12 11 13 13 15 14 10

chain nodes : 6 7 8 10 16 ring nodes :

1 2 3 4 5 11 12 13 14 15 18 19 20 21 22 23

chain bonds :

1-10 6-7 6-8 7-11 7-16 12-18

ring bonds :

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-16 11-12 11-15 12-13 13-14 14-15

exact bonds :

12-18

normalized bonds :

18-19 18-23 19-20 20-21 21-22 22-23

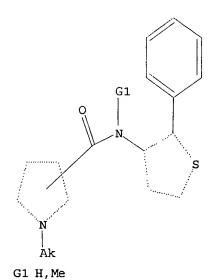
G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom 16:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom

L4 STRUCTURE UPLOADED

=> d 14 L4 HAS NO ANSWERS L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 12:03:05 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 68 TO 532
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s 14 full

FULL SEARCH INITIATED 12:03:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 469 TO ITERATE

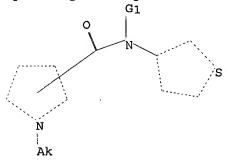
100.0% PROCESSED 469 ITERATIONS 6 ANSWERS

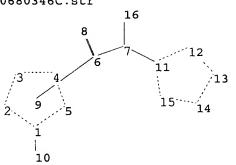
SEARCH TIME: 00.00.01

L6 6 SEA SSS FUL L4

=>

Uploading C:\Program Files\Stnexp\Queries\10680346C.str





chain nodes : 6 7 8 10 16 ring nodes :

1 2 3 4 5 11 12 13 14 15

chain bonds :

1-10 6-7 6-8 7-11 7-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

 $1-2 \quad 1-5 \quad 1-10 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-8 \quad 7-11 \quad 7-16 \quad 11-12 \quad 11-15 \quad 12-13 \quad 13-14 \quad 14-15$

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom 16:CLASS

L7 STRUCTURE UPLOADED

=> s 17

SAMPLE SEARCH INITIATED 12:04:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 940 TO ITERATE

100.0% PROCESSED 940 ITERATIONS 11 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 16961 TO 20639 PROJECTED ANSWERS: 22 TO 418

L8 11 SEA SSS SAM L7

=> s 17 full

FULL SEARCH INITIATED 12:04:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17912 TO ITERATE

100.0% PROCESSED 17912 ITERATIONS 243 ANSWERS

SEARCH TIME: 00.00.01

L9 243 SEA SSS FUL L7

=> fil caplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 487.43 487.64

FILE 'CAPLUS' ENTERED AT 12:05:19 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 19

L10 22 L9

=> d ed abs ibib hitstr 110

L10 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 07 Apr 2005

The invention relates to quinazoline derivs. I [R2 or the substituted pyrrolidinyloxy group is in the 6 or 7 position of the quinazoline ring; A is Ph or pyridyl: m is 0-3; n is 0-2; R1 is halo, cyano, nitro, hydroxy, carboxy, trifluoromethyl, alkyl, alkoxy, alkylsulfonyl, alkylureido, etc.: R2 is H, alkyl, cycloalkyl, cycloalkylalkyl or (un)substituted alkoxy: R3 is H, alkyl, cycloalkyl, alkylsulfinyl, carbamoylalkyl, etc.: R4 is alkyl, alkoxy, cyano, halo, hydroxy or oxo: R5 is H or alkyl: R6 is H, alkyl, alkoxy, heterocyclyl, heterosycly, etc.: or R5RGN is a ringl, including processes for their preparation, pharmaceutical compns. containing.

, and their use as antiproliferative agents in the prevention or treatment of tumors which are sensitive to inhibition of erbB receptor tyrosine kinases. Thus, compound II was prepared by etherification of Boc-protected cia-4-hydroxy-D-proline Me ester with 4-chloro-7-methoxyquinazolin-6-ol and reaction of the product with 3-chloro-2-fluoroannilne in 4.0 M HCL/dioxane and acetonitrile, followed by reductive N-methylation, nification.

HCI/dioxane and acetonitrile, followed by requestive nomes, asponification, and amidation. Compound II showed IC50 = 0.008 nM for inhibition of EGFR tyrosine kinase protein phosphorylation and IC50 = 0.144 nM in the EGFR driven KB cell proliferation assay.

ACCESSION NUMBER: 2005:300434 CAPLUS
DOCUMENT NUMBER: 142:374111

TITLE: Preparation of proline quinazoline derivatives as antiproliferative agents
INVENTOR(S): Bradbury, Robert Hugh; Halsall, Christopher Thomas; Hennequin, Laurent Francois Andre; Kettle, Jason Grant; Plowright, Alleyn

L10 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
PATENT ASSIGNEE(S):
SOURCE:
PTT Int. Appl., 198 pp.
CODEN: PIXXD2

DOCUMENT TYPE:
Patent
Spain

English 2

PATE	NT I	NO.			KIN	2	DATE			APPL	ICAT	ION	NO.		D.	ATE	
						-								-	-		
WO 2	005	0307	57		A1		2005	0407		WO 2	004-	GB40	85		2	0040	922
1	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	co,	CR,	Cυ,	CZ,	DE,	DK,	DM,	DŽ,	EC,	EÉ,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ÍD,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG,	SK,	SL,	SY,
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1	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	52,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	ÐΚ,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN.	TD.	ŤG													

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 142:374111
IT 849345-53-59
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of proline quinazoline derivs. as antiproliferative agents) 849345-53-5 CAPLUS

849343-33-3 CAPLUS 2-Pyrrolidinecarboxamide, 4-[[4-[(3-chloro-2-fluorophenyl)amino]-7-methoxy-6-quinazolinyl]oxy]-1-methyl-N-3-thienyl-, (2R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ed abs ibib hitstr 1-22

ANSWER 1 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 07 Apr 2005

The invention relates to quinazoline derivs. I [R2 or the substituted pyrrolidinyloxy group is in the 6 or 7 position of the quinazoline ring; A is Ph or pyridyl; m is 0-3; n is 0-2; R1 is halo, cyano, nitro, hydroxy, carboxy, trifluoromethyl, alkyl, alkoxy, alkylsulfonyl, alkylureido, etc.; R2 is H, alkyl, cycloalkyl, cycloalkyl, alkylthio, alkylsulfinyl, carbamoylalkyl, etc.; R4 is alkyl, eloxy, cyano, halo, hydroxy or oxo: R5 is H or alkyl; R6 is H, alkyl, alkoxy, theterocyclyl, heteroaryl, etc.; or R5R6N is a ringl, including processes for their preparation, pharmaceutical compns. containing

and their use as antiproliferative agents in the prevention or treatment of tumors which are sensitive to inhibition of crbB receptor tyrosine kinases. Thus, compound II was prepared by etherification of Boc-protected cis-4-hydroxy-D-proline Me ester with 4-chloro-7-methoxyquinazolin-6-ol and reaction of the product with 3-chloro-2-fluoroanniline in 4.0 M HCl/dioxane and acetonitrile, followed by reductive N-methylation, nification, saponification,

nification, Compound II showed IC50 = 0.008 nM for inhibition of EGFR tyrosine kinese protein phosphorylation and IC50 = 0.144 nM in the EGFR driven KB cell proliferation assay.

SION NUMBER: 2005: 300434 CAPLUS (EMT) NUMBER: 142:374111

ACCESSION NUMBER:

DOCUMENT NUMBER: TITLE:

. INVENTOR (S):

Preparation of proline quinazoline derivatives as antiproliferative agents Bradbury, Robert Hugh; Halsall, Christopher Thomas; Hennequin, Laurent Francois Andre; Kettle, Jason Grant: Playright, Billeyn

Grant; Plowright, Alleyn

ANSWER 2 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 24 Sep 2004 L10

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Sulfonamide lactams of formula 1 (wherein X = (un)substituted (CH2)m; m = 1-3; R1 = (un)substituted alk(en/yn)yl, cycloalkyl, hetero/aryl, cyclohetezoalkyl; R2, R3 = independently H, (un)substituted alk(en/yn)yl, cycloalkyl, hetero/aryl, cycloalkyl, hetero/aryl, cycloalkyl, hetero/aryl, cycloalkyl, hetero/aryl, cycloalkyl, R6, R4a, R5, R5a = independently H, OH, alkoxy, CO2H and derivs., CONH2 and derivs., S(O)qH and derivs., SO2H2 and derivs., etc. (un)substituted alk(en/yn)yl, cycloalkyl, hetero/aryl, cycloheteroalkyl; q = 0-2; R6, R6a = independently H, (un)substituted alk(en/yn)yl, cycloalkyl, substituted (CH2)n-H or R7NR8 = (un)substituted alk(en/yn)yl, cycloalkyl, substituted (CH2)n-H or R7NR8 = (un)substituted cycloheteroalkyl; n = 1-4; with the proviso that certain compds. are absent; their pharmaceutically acceptable salts, stereoisomers and prodrugs| were prepared as inhibitors of Factor X, and useful as anticoagulants in the treatment of cardiovascular diseases associated with thromboses (no data). For instance, reacting amine II with naphthalene-2-sulfonyl chloride in CH2C12 in the presence of TEA for 30 min at room temperature gave sulfonamide III in 66t yield.

ACCESSION NUMBER: 2004:780362 CAPLUS

DOCURENT NUMBER: 141:295864

Preparation of sulfonamide lactams as Factor Xa inhibitors

Preparation of sulfonamide lactams as Factor Xa inhibitors O'Connor, Stephen P.: Lawrence, Michael; Shi, Ya INVENTOR (S):

O'Connor, Stephen P.; Lawrence, Michael; Shi, Yan; Stein, Philip D.

PATENT ASSIGNEE(S): SOURCE: U.S. Pat. Appl. Publ., 257 pp. CODEN: USXXCO

DOCUMENT TYPE: LANGUAGE: Patent

English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE 20040923 US 2004186134 A1 US 2003-374299 20030226 PRIORITY APPLN. INFO.: OTHER SOURCE(S): IT 445277-00-9P US 2003-374299 MARPAT 141:295864

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(drug candidate; preparation of sulfonamide lactams as factor Xa inhibitors and anticoagulants)
445277-00-9 CAPLUS
2-Pyrrolidinecarboxamide, 1-[[3S]-3-[[(1E]-2-(5-chloro-2-thleny)]sulfony]]amino]-2-oxo-1-piperidiny]]acety]]-N-(tetrahydro-1,1-dioxido-3-thieny])-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

. .

Page 1030/08/2005

L10 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continu-PATENT ASSIGNEE(S): Astrazeneca AB, Swed.: Astrazeneca UK Ltd. SOURCE: PTT Int. Appl., 198 pp.

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE 20050407 WO 2005030757 A1 WO 2004-GR4085 20040922

GB 2003-22409 GB 2003-22534 PRIORITY APPLN. INFO.: A 20030925 A 20030926

OTHER SOURCE(S): IT 849345-53-5P MARPAT 142:374111

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

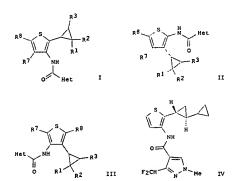
(preparation of proline quinazoline derivs. as antiproliferative agents) 849345-53-5 CAPLUS 2-Pyrrolidinecarboxamide, 4-[[4-[(3-chloro-2-fluorophenyl)amino]-7-methoxy-6-quinazolinyl]oxy]-1-methyl-N-3-thienyl-, (2R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT REFERENCE COUNT:

L10 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 13 May 2004



A fungicidally active compound I, II, or III (wherein Het = (un)substituted 5- or 6-membered heterocyclic ring containing one to three O, N, and/or S atoms, provided that the ring is not 1,2,3-triazole; Rl and R2 = independently H, halo, or Me; R3 = (un)substituted (cyclo)alkyl, alkenyl, alkynyl, Ph, heterocyclyl; R7 and R8 = independently H, halo, or (halo)alkyl) were prepared for use as active ingredients in agricultural or hotticultural compns. for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. For example, 3-difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid was amidated with [2-(bicyclopropyl-2-yl)thiophen-3-yl]amine in the presence of TEA and N,N-bis(2-oxooxazolidinyl)phosphinic acid chloride in CH2Cl2 to give trans-IV [97k purity]. The latter showed excellent activity against Puccinia recondita on wheat (0-5% infestation) and showed good activity against Podosphaera leucotricha on apple, Venturia inaequalis on apple, Erysiphe graminis on barley, Pyrenophora teres on barley, Alternaria solani on tomato, and Uncinula necator on grape (<20% infestation for second

each). ACCESSION NUMBER: 2004:390242 CAPLUS 140:406731

DOCUMENT NUMBER: TITLE: Preparation of N-(cyclopropylthienyl)carboxamides as

fungicides

Ehrenfreund, Josef; Tobler, Hans; Walter, Harald Syngenta Participations Ag, Switz. PCT Int. Appl., 43 pp. CODEN: PIXXD2 INVENTOR(S): PATENT ASSIGNEE(S):

SOURCE:

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN 688325-83-9P 688325-84-0P 688325-88-4P 688325-88-4P 688325-89-2P 688325-98-73 688325-89-4P 688325-99-8P 688325-99-8P 688325-99-4P 688325-99-4P 688325-93-1P 688325-94-2P 688325-93-1P 688325-94-2P 688325-99-4P 688325-96-3P 688325-96-3P 688325-96-3P 688325-96-3P 688326-03-5P 688326-03-6P 688326-03-6P 688326-01-8P 688326-02-5P 688326-10-5P 688326-10-5P 688326-10-5P 688326-10-5P 688326-10-5P 688326-11-2P 688326-11-2P 688326-11-2P 688326-11-2P 688326-11-2P 688326-11-2P 688326-12-1P 688326-11-2P 688326-11-2P 688326-21-1P 688326-11-2P 688326-21-1P 688326-21P 688326-21-1P 688326-21-1P 688326-21-1P 688326-21-1P 688326-(Continued)

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES

(Sungicide; prepn. of N-(cyclopropylthienyl)carboxamides as fungicides) 688322-46-5 CAPLUS
H-Pyrrole-3-carboxamide, N-[2-(2-ethylcyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-47-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-{2-ethylcyclopropyl}-3-thienyl}-1(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-48-7 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-(2-propylcyclopropyl)-3-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN
DOCUMENT TYPE: Patent
LANGUAGE: English
FANILY ACC. NUM. COUNT: 1 '(Continued)

PATENT NO. KIND DATE APPLICATION NO. DATE ENT NO. KIND DATE APPLICATION NO. DATE

2004039799 A1 20040513 W0 2003-EP11805 20031024
W: AB, AG, AL, AM, AT, AU, AZ, BA, BB, BB, GB, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, NM, MM, MX, MZ, NI, NO, NZ, CM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CM, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
2501739 AA 20040513 CA 2003-2501739 20031024
B1556377 A1 20050727 EP 2003-776869 20031024
B1 20050727 EP 2003-776869 20031024
B1 20150728 B2 2003-25554 A2 20021101
B1 WARPAT 140:406731 WO 2004039799 GH, GM, LR, LS, OM, PG, TN, TR, RW: GH, GM, KG, KZ, FI, FR, BF, BJ, CA 2501739 EP 1556377

PRIORITY APPLN. INFO.:

PRIORITY APPLN. INFO.:

OTHER SOURCE(S):

MARPAT 140:406731

IT 689322-46-59 669322-47-69 689322-46-79 689322-49-89 669322-55-19 689322-55-27 689322-55-27 689322-55-29 689322-55-49 689322-55-59 689322-55-69 689322-55-69 689322-55-69 689322-56-59 689322-56-59 689322-66-39 689322-66-39 689322-66-39 689322-66-39 689322-66-39 689322-67-09 689322-76-79 689322-77-29 689322-73-89 689322-73-89 689322-73-89 689322-73-89 689322-73-89 689322-73-89 689322-73-89 689322-73-89 689322-73-89 689322-73-89 689322-73-99 689322-73-99 689322-73-99 689322-73-99 689322-73-99 689322-73-99 689322-73-99 689322-73-99 689322-73-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689322-99-99 689323-06-99 689323-06-99 689323-06-99 689323-06-99 689323-06-99 689323-06-99 689323-06-99 689323-06-99 689323-06-99 689323-06-99 689323-11-79 689323

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

688322-49-8 CAPLUS
1H-Pyrrole-3-carboxamide, 4-{difluoromethyl}-1-methyl-N-{2-{2-propylcyclopropyl}-3-thienyl}- {9CI} (CA INDEX NAME)

688322-50-1 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-[2-(1-methylethyl)cyclopropyl]-3thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-51-2 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-[2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

688322-52-3 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-{2-[2-(1-methylethyl)cyclopropyl]-3-thlenyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

1-Pr.

RN 688322-53-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[2-[2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

i-Pr O II C-NH

RN 688322-54-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1-ethyl-4-methyl-N-[2-[2-[1-methylethyl]cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

i-Pr O C-NH

RN 688322-55-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1, 4-dimethyl-N-[2-[2-[1-methylethyll-yclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continue

n-Bu

O

C-NH

CF3

RN 688322-59-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-butylcyclopropyl)-3-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me N C- NH S

RN 688322-60-3 CAPLUS
CN 1H-Pyrclola-3-carboxamide, N-[2-(2-butylcyclopropyl)-3-thienyl]-2-fluoro1,4-dimethyl- (9C1) (CA INDEX NAME)

Me O C-NH-S

RN 688322-61-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-butylcyclopropyl)-3-thienyl]-2-chloro1,4-dimethyl- (9C1) (CA INDEX NAME)

RN 688322-62-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-{2-[2-(2-methylpropyl)cyclopropyl}-3-

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L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688322-56-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-ethyl-2-fluoro-4-methyl-N-[2-{2-{1-methyl-tyl-pyclopropyl}-3-thienyl}- (9CI) (CA INDEX NAME)

Me O C NH

RN 688322-57-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-{chlorodifluoromethyl}-2-fluoro-1-methyl-N-[2[2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

C1-CF2 0 | C-NH-S

RN 688322-58-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-butylcyclopropyl)-3-thienyl]-1-methyl-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

1-Bu
0
1-Bu
0
C-NH

RN 688322-63-6 CAPLUS
CN IN-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-[2-(2-methylpropyl)gropyl)-3-thienyl)- (9Ci) (CA INDEX NAME)

1-Bu 0 1-Bu C-NH

RN 668322-64-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-[2-[2-[2-(2-methylpropyl)cyclopropyl]-3-thienyl]- (9C1) (CA INDEX NAME)

i-Bu

O

C-NH

RN 688322-65-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(methoxymethyl)-N-[2-[2-(2-methylpropyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

1-BU 0 C-NH CF3

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688322-66-9 CAPLUS
1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[2-[2-(2-methylpropyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

688322-67-0 CAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[2-[2-[2-methylpropyl]cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

688322-68-1 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-[2-[1,1-dimethylethyl)cyclopropyl]-3thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-69-2 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[2-{2-(1,1-dimethylcyclopropyl]-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

688322-73-8 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-(2-pentylcyclopropyl)-3-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-74-9 CAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-[2-(3-methylbutyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-75-0 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-[2-(3-methylbutyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

688322-76-1 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(2-hexylcyclopropyl)-3-thienyl]-1-methyl-4-

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L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688322-70-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-[2-{1,1-dimethylethyl}cyclopropyl]-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

688322-71-6 CAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-N-[2-[2-[1,1-dimethylethyl]cyclopropyl]-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

688322-72-7 CAPLUS
IH-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[2-[2-[1,1-dimethylethyl)cyclopropyl]-3-thlenyl]-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-77-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-{1,1'-bicyclopropyl}-2-yl-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688322-78-3 CAPLUS 1H-Pyrrole-3-carboxamide, N-(2-{1,1'-bicyclopropyl}-2-yl-3-thienyl)-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688322-79-4 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-{1,1'-bicyclopropyl}-2-yl-3-thienyl}-2-fluoro-1,4-dimethyl- (9C1) (CA INDEX NAME)

688322-80-7 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-[1,1'-bicyclopropyl]-2-yl-3-thienyl)-2-chloro-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688322-81-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-{2-cyclobutylcyclopropyl}-3-thienyl}-1methyl-4-{trifluoromethyl}- (9CI) (CA INDEX NAME)

RN 688322-82-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclobutylcyclopropyl)-3-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me C-NH S

RN 688322-83-0 CAPLUS
CN 1H-Fyrrole-3-carboxamide, N-{2-{2-cyclopentylcyclopropyl}-3-thienyl}-1methyl-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 688322-86-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[2-(2-cyclopentylcyclopropyl)-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 688322-87-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclopentylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9C1) (CA INDEX NAME)

Me CONTRACTOR

RN 688322-88-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-[2-(2-cyclopentylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688322-84-1 CAPLUS CN 1H-Pytrole-3-carboxamide, N-(2-(2-cyclopentylcyclopropyl)-3-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688322-85-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclopentylcyclopropyl)-3-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688322-89-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclohexylcyclopropyl)-3-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688322-90-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cyclohexylcyclopropyl)-3-thienyl]-4(diffuoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688322-91-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(2-cyclohexylcyclopropyl)-3-thienyl}-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me N CH2F

RN 688322-92-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[2-(2-cyclohexylcyclopropyl)-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

Me N C- NH CF2-C1

RN 688322-93-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(3-cyclohexyl-2,2-difluorocyclopropyl)-3-thienyl}-1-methyl-4-(trifluoromethyl)- {9CI} (CA INDEX NAME)

Me C-NH S

RN 688322-94-3 CAPLUS
CN H-Fyrrole-3-carboxamide, N-[2-(2-cyclohexylcyclopropyl)-3-thienyl]-2fluoro-1,4-dimethyl- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 688322-98-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cycloheptylcyclopropyl)-3-thlenyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688322-99-8 CAPLUS
CN IH-Pyrrole-3-carboxamide, N-[2-[2-cycloheptylcyclopropyl]-3-thienyl]-4(fluoromethyl]-1-methyl- [9CI] (CA INDEX NAME)

RN 688323-00-4 CAPLUS

(N IN-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-(2-(2-cycloheptylcyclopropyl)-3-thienyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688323-01-5 CAPLUS
CN | H-Pyrrole-3-carboxamide, N-(2-(2-cycloheptylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688322-95-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-(2-(2-cyclohexylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688322-96-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cycloheptylcyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688322-97-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(2-cycloheptylcyclopropyl)-3-thienyl]-1-ethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Contin

RN 688323-02-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-[Z-(2-cycloheptylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688323-03-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-(2-cyclooctylcyclopropyl)-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688323-04-8 CAPLUS
CN 1H-Pyzrole-3-carboxamide, N-[2-(2-cyclooctylcyclopropyl)-3-thienyl]-4(diffuoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688323-05-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-{2-(2-phenylcyclopropyl)-3-thienyl}-4-

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (trifluoromethyl) - (9CI) (CA INDEX NAME)

RN 688323-06-0 CAPLUS
CN | H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-(2-phenylcyclopropyl)-3-chienyl]- (9CI) (CA INDEX NAME)

RN 688323-07-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-[2-(2-phenylcyclopropyl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688323-08-2 CAPLUS
CN IN-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[2-(2-phenylcyclopropyl)-3-thienyl]- (9Cl INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-12-8 CAPLUS
CN IM-Pyrrole-3-carboxamide, N-[2-[2-(4-chlorophenyl)cyclopropyl]-3-thienyl]l-methyl-4-(trifluoromethyl)- (SCI) (CA INDEX NAME)

RN 688323-13-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-[2-(4-chloropheny1)cyclopropy1]-3-thieny1]4-(difluoromethyl)-1-methy1- (9CI) (CA INDEX NAME)

RN 688323-14-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-[2-(4-bromophenyl)cyclopropyl]-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-09-3 CAPLUS
CN H-Pytrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[2-(2-phenylcyclopropyl)-3-thlenyl]- (9C1) (CA INDEX NAME)

RN 688323-10-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-[2-(4-fluorophenyl)cyclopropyl]-3-thienyl]1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688323-11-7 CAPLUS
CN IH-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[2-(2-(4-fluorophenyl)cyclopropyl]-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-15-1 CAPLUS
CN 1H-Fyrrole-3-carboxamide, N-[2-[2-(4-bromopheny1)cyclopropy1]-3-thieny1]-4(difluoromethy1)-1-methy1- (9CI) (CA INDEX NAME)

RN 688323-16-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-[2-(2-thienyl)cyclopropyl]-3-thienyl]-4-trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688323-17-3 CAPLUS
CN 1H-Pyrcle-3-carboxamide, 1-methyl-N-[2-{2-(3-thienyl)cyclopropyl}-3-thienyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-18-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-[2-(2-furanyl)cyclopropyl]-3-thienyl]-1methyl-4-(triflurormethyl)- (9CI) (CA INDEX NAME)

F3C NH

RN 688323-19-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-[2-(3-furany1)cyclopropy1]-3-thieny1]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

F3C CON NH

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688325-61-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-ethylcyclopropyl)-3-thienyl]-1-methyl-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me N C-NH S

RN 688325-62-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-ethylcyclopropyl)-3-thienyl)-1(methoxymethyl)-4-trifluoromethyl)- (9CI) (CA INDEX NAME)

MeO-CH2 N C-NH S

RN 688325-63-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-(2-propylcyclopropyl)-3-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

He CF3

RN 688325-64-6 CAPLUS

N 1H-Pyrrole-3-carboxemide, 4-(difluoromethyl)-1-methyl-N-[4-(2-propylcyclopropyl)-3-thienyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688323-20-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[2-(1'-methyl[1,1'-bicyclopropyl]-2-y1)-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me N C NH S

RN 688323-21-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[2-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-3-thienyl]- (9CI) (CA INDEX NAME)

Me C-NH S

RN 688323-22-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[2-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-3-thienyl]- (9CI) (CA INDEX NAME)

Me O C NH S

RN 688323-23-1 CAPLUS
CN 1H-Pyrclo1-3-carboxemide, 2-chloro-1,4-dimethyl-N-{2-(1'-methyl{1,1'-bicyclopropyl]-2-yl)-3-thienyl]- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me O O C O NH S

RN 688325-66-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(1-methylethyl)cyclopropyl]-3thlenyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me N CF3

RN 688325-67-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-{4-{2-(1-methyl-thyl)cyclopropyl)-3-thienyl}- (9CI) (CA INDEX NAME)

Me O S C-NH S

RN 688325-68-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-[4-[2-(1-methyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

Me N C-NH S
CH₂F

RN 688325-69-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[4-{2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me O C NH C NH Pr-

RN 688325-70-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1-ethyl-4-methyl-N-[4-[2-(1-methylethyl)cyclopropyl]-3-thienyl}- (9CI) (CA INDEX NAME)

RN 688325-71-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[4-[2-(1-methyl-thyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688325-72-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-ethyl-2-fluoro-4-methyl-N-[4-[2-{1-methyl-tyl}cyclopropyl]-3-thienyl]- [9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 688325-76-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-butylcyclopropyl)-3-thienyl]-2-fluoro1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688325-77-1 CAPLUS
CN HH-Pyrrole-3-carboxamide, N-[4-(2-butylcyclopropyl)-3-thienyl]-2-chloro1,4-dimethyl- (9CI) (CA INDEX NAME)

Me O II C-NH-S

RN 688325-78-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(2-methylpropyl)cyclopropyl]-3thienyl]-4-(trifuoromethyl)- (9CI) (CA INDEX NAME)

Me N CF3

RN 688325-79-3 CAPLUS
CN H-Pyrcole-3-carboxamide, 4-(difluoromethyl)-1-methyl-n-[4-[2-(2-methyl)propyl)pyclopropyl]-3-thienyl]- (9C1) (CA INDEX NAME)

Me N C-NH S
CHF2
Bu-i

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688325-73-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-2-fluoro-1-methyl-N-[4{2-(1-methylethyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688325-74-8 CAPLUS
CN | H-Pyrrole-3-carboxamide, N-[4-(2-butylcyclopropyl)-3-thienyl]-1-methyl-4(trifluoromethyl)- (9C1) (CA INDEX NAME)

Me CF3

RN 688325-75-9 CAPLUS CN 1H-Pyrrole-3-carboxamide, N-[4-(2-butylcyclopropyl)-3-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me N CHF2 S

LIO ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 688325-80-6 CAPLUS
CN IM-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-[4-[2-(2-methylpropyl)cyclopropyl]-3-thienyl]- (9CI) (CA INDEX NAME)

Me O C-NH-S
CH2F

RN 688325-81-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(methoxymethyl)-N-[4-[2-(2-methylpropyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

MeO-CH2 N C-NH S

RN 688325-82-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-(4-[2-[2-methylpropyl)cyclopropyl]-3-thlenyl]- (9C1) (CA INDEX NAME)

RN 688325-83-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[4-[2-(2-methylpropyl)cyclopropyl]-3-thienyll- (9CI) (CA INDEX NANE)

Me O C NH S

LIO ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 688325-84-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-[2-(1,1-dimethylethyl)cyclopropyl)-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688325-85-1 CAPLUS
CN IH-Pytrole-3-carboxamide, 4-(difluoromethyl)-n-{4-[2-(1,1-dimethylethyllcyclopropyl]-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 688325-86-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-[2-(1,1-dimethylethyl)cyclopropyl]-3-thiopyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688325-87-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-[4-[2-(1,1-dimethylethyl)cyclopropyl)3-thienyl=1,4-dimethyl- (9C1) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[4-[2-(3-methylbutyl]-cyclopropyl]-3-thienyl]- (SCI) (CA INDEX NAME)

RN 688325-92-0 CAPLUS
CN HH-Fyrrole-3-carboxamide, N-(4-(2-hexylcyclopropyl)-3-thienyl)-1-methyl-4(trifluoromethyl)- (SCI) (CA INDEX NAME)

RN 688325-93-1 CAPLUS
CN IM-Pyrrole-3-carboxamide, N-(4-[1,1'-bicyclopropyl]-2-yl-3-thienyl)-1methyl-4-(trifluoromethyl)- (SCI) (CA INDEX NAME)

RN 688325-94-2 CAPLUS
CN IN-Pyrcole-3-carboxamide, N-(4-[1,1'-bicyclopropyl]-2-yl-3-thienyl)-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688325-95-3 CAPLUS
CN lH-Pyrrole-3-carboxamide, N-(4-[1,1'-bicyclopropyl]-2-yl-3-thienyl)-2-fluoro-1,4-dimethyl- (SCI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 688325-88-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-{4-{2-(1,1-dimethylethyl)cyclopropyl}-3-thienyl}-1-methyl- {9Cl} (CA INDEX NAME)

RN 688325-89-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-pentylcyclopropyl]-3-thienyl]-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688325-90-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(3-methylbutyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688325-91-9 CAPLUS

LIO ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688325-96-4 CAPLUS CN 1H-Pyrrole-3-carboxamide, N-{4-{1,1'-bicyclopropyl}-2-yl-3-thienyl}-2chloro-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688325-97-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-cyclobutylcyclopropyl)-3-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688325-98-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-cyclobutylcyclopropyl)-3-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688325-99-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

LIO ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688326-00-3 CAPLUS 1H-Pyrole-3-carboxamide, N-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-4-(difluoromethyl)-1-methyl- (SCI) (CA INDEX NAME)

688326-01-4 CAPLUS
1H-Pyrrole-3-carboxamide, N-{4-(2-cyclopentylcyclopropyl)-3-thienyl}-4-(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688326-05-8 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-{2-cyclohexylcyclopropyl)-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688326-06-9 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclohexylcyclopropyl)-3-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

688326-07-0 CAPLUS
1H-Pyrrole-3-carboxamide, N-{4-(2-cyclohexylcyclopropyl)-3-thienyl}-4-(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Page 2030/08/2005

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688326-02-5 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[4-{2-cyclopentylcyclopropyl}-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

688326-03-6 CAPLUS
IH-Pyrrole-3-carboxamide, N-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9C1) (CA INDEX NAME)

688326-04-7 CAPLUS IM-Pyrrole-3-carboxamide, 2-chloro-N-[4-(2-cyclopentylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 688326-08-1 CAPLUS
CN | H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-{4-(2cyclohexylcyclopropyl)-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

688326-09-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-{4-(3-cyclohexyl-2,2-difluorocyclopropyl)-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688326-10-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-[4-(2-cyclohexylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

688326-11-6 CAPLUS
1H-Pyrrole-3-carboxamide, 2-chloro-N-[4-(2-cyclohexylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

688326-12-7 CAPLUS

L10 ANSMER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN H-Pyrrole-3-carboxamide, N-{4-(2-cycloheptylcyclopropyl)-3-thienyl]-1methyl-4-(trifluoromethyl)-(951) (CA INDEX NAME)

RN 688326-13-8 CAPLUS
CN 1H-Pytrole-3-carboxamide, N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-1-ethyl-4-ttrifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-15-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688326-16-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688326-21-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{4-(2-cyclooctylcyclopropyl)-3-thienyl}-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688326-22-9 CAPLUS
CN lH-Pyrcole-3-carboxamide, 1-methyl-N-[4-(2-phenylcyclopropyl)-3-thienyl]-4[trifluoromethyl)- (9CT) (CA INDEX NAME)

RN 688326-23-0 CAPLUS
CN 1H-Pyrcole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[4-(2-phenylcyclopropyl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688326-24-1 CAPLUS
CN 1H-Pytrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-{4-(2-phenyleyclopropyl)-3-thienyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688326-17-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-2-fluoro-1-methyl- (9CI) (CA INDEX NAME)

.RN 688326-18-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-2-fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688326-19-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-[4-(2-cycloheptylcyclopropyl)-3-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688326-20-7 CAPLUS
CN IM-Pyrrole-3-carboxamide, N-[4-(2-cyclooctylcyclopropyl)-3-thienyl]-1methyl-4-(trifluoromethyl)- (9Cl) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688326-25-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-[4-(2-phenylcyclopropyl)-3-thenyl-(9C1) (CA IMDEX NAME)

RN 688326-26-3 CAPLUS
CN H-Pyrcole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[4-{2-phenylcyclopropyl}-3-thlenyl]- (901) (CA INDEX NAME)

RN 688326-27-4 CAPLUS
CN | H-Pyrrole-3-carboxamide, N-[4-[2-(4-fluorophenyl)cyclopropyl]-3-thienyl]|-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-28-5 CAPLUS

CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[4-[2-[4-fluorophenyl]cyclopropyl]-3-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me N CHF2

RN 688326-29-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{4-[2-(4-chlorophenyl)cyclopropyl]-3-thienyl]1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me N CF3

RN 688326-30-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-[2-(4-chlorophenyl)cyclopropyl]-3-thienyl]4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me CHF2

RN 688326-31-0 CAPLUS
CN lH-Pyrrole-3-carboxamide, N-[4-[2-(4-bromophenyl)cyclopropyl]-3-thienyl]-1methyl-4-(trifluromethyl)- (9CI) (CA INDEX NAME)

Me N C-NH S

RN 688326-32-1 CAPLUS CN 1H-Pyrrole-3-carboxamide, N-[4-[2-(4-bromophenyl)cyclopropyl]-3-thienyl]-4-

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

F3C CON NH

RN 688326-36-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-[2-(3-furany1)cyclopropy1]-3-thieny1]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688326-37-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-3-thienyl]-4-(trifluoromethyl)- (9cI) (CA INDEX NAME)

Me N C-NH S

RN 688326-38-7 CAPLUS

CN IH-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[4-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-3-thienyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

Me N CHF2

RN 688326-33-2 CAPLUS
CN IH-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(2-thienyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

F3C C== C

RN 688326-34-3 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[4-[2-(3-thienyl)cyclopropyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

F₃C C O

RN 688326-35-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{4-{2-(2-furanyl)cyclopropyl}-3-thienyl}-1-methyl-4-(trifiuoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Me O CHF2

RN 688326-39-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-(4-(1'-methyl(1,1'-bicyclopropyl)-2-yl)-3-thienyl]- (9CI) (CA IMDEX NAME)

Me O C NH S

RN 688326-40-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-(4-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-3-thienyl]- (9CI) (CA INDEX NAME)

RN 688328-21-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-{2-[(1R,2R)-2-(1,1-dimethylethyl)cyclopropyl}-3-thienyl}-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

 $688328-22-5 \quad CAPLUS \\ 1H-Pyrrole-3-carboxamide, N-[2-(1R,2S)-[1,1'-bicyclopropyl]-2-yl-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9C1) (CA INDEX NAME)$

Relative stereochemistry.

688328-23-6 CAPLUS
IH-Pyrole-3-carboxamide, N-[2-[(IR,2R)-2-(4-fluorophenyl)cyclopropyl)-3-thienyl]-I-methyl-4-(trifluoromethyl)-, rel- [9C] (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 14 Apr 2004

AB DNA binding ligands with potent antimicrobial activity against Gram-pos.
bacteria were further optimized by variation of the internal aromatic amino
acids. This modification led to compds. with improved in vivo efficacy in
lethal murine models of peritonitis (methicillin-resistant 5. aureus,
MRSA) and lung infection (5. pneumoniae).

ACCESSION NUMBER: 2004:30252 CAPLUS

DOCUMENT NUMBER: 141:64377

DNA binding ligands with in vivo efficacy in murine
models of bacterial infection: optimization of
internal aromatic amino acids

Burli, Roland W.; Kaizeman, Jacob A.; Duan, Jian-Xin;
Jones, Peter: Johnson, Kirk W.; Iwamoto, Mari: Truong,
Kiet: Hu, Wenhao: Stanton, Timothy; Chen, Alfred:
Touami, Sofia; Gross, Matthew; Jiang, Vernon; Ge,
Yigong; Moser, Heinz E.
Genesoft Pharmaceuticals, South San Francisco, CA,
94080, USA

Bioorganic & Medicinal Chemistry Letters (2004),
14(9), 2067-2072
CODEN: EMCLES; ISSN: 0960-894X

Elsevier Science B.V.

DOCUMENT TYPE: Journal
LANGUAGE: Enclish

DOCUMENT TYPE: LANGUAGE: IT 710950-17-7 Journal English

710950-17-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(DNA binding ligands with in vivo efficacy in murine models of
bacterial infection and structure-activity relationship)
710950-17-7 CAPLUS
3-Isoquinolinecarboxamide, N-[1-methyl-5-[[[5-[[[1-methyl-5-[[[2-(4-morpholiny)]+ethyl]amino]carbonyl]-1H-pyrrol-3-yl]amino]carbonyl]-3thienyl]amino]carbonyl]-1H-pyrrol-3-yl]- (9CI) (CA INDEX NAME)

PAGE 1-B

REFERENCE COUNT:

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

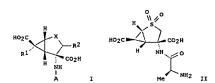
688328-24-7 CAPLUS coos.zd=z4=/ CAPLUS
H=Pyrrole-3-carboxamide, N={2-{(1R,2R)-2-{4-chlorophenyl)cyclopropyl}-3thienyl}-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 21 Dec 2003



AB The invention relates to synthetic excitatory amino acid prodrugs for the treatment of neurol. disorders and psychiatric disorders. Bicyclic amino acids I (A is H-Q1-10, where Q is aminoacyl; X is O, S, SO, SO2, or aubstituted methylene; RI is H or F: R2 is H, F, or OH) or their pharmaceutically-acceptable salts are claimed. Thus, prodrug II.HCl was prepared via peptide coupling reaction and shown to exhibit comparable concentration in rat plasma to that of the non-prodrug form.

ACCESSION NUMBER: 2003:991499 CAPLUS
DOCUMENT NUMBER: 140:42463
ITILE: Preparation of prodrugs of excitatory amino acids INVENTOR(S): Moher, Eric David; Monn, James Allen; Pedregal-Tercero, Concepcion

PATENT ASSIGNEE(S): Eli Lilly and Company, USA; Collado, Cano Ivan; Blanco-Utgoiti, Jamie Gonzalo

SOURCE: PITIL APPLI, 172 pp.
CODEN: PITXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC, NUM. COUNT: 1
PATENT INFORMATION:

PR

PAT	ENT	ΝО.			KIN	D	DATE			APPL	ICAT:	ION	NO.		D	ATE	
						-											
WO	2003	1042	17		A2		2003	1218	1	WO 2	003-1	US 15	105		21	0030	606
WO	2003	1042	17		A3		2004	0226									
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		co,	CR,	Cυ,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	15,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,
		TZ,	UA,	UG,	US,	υz,	vc,	VN,	YU,	ZA,	ZM,	ZW					
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		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	£Ε,	ES,
		FI,	FR,	GB,	GR,	ΚU,	IE.	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
CA	2488	167			AA		2003	1218		CA 2	003-	2488	167		21	0030	606
EP	1517	915			A2		2005	0330	1	EP 2	003-	7572	66		21	0030	606
	R:	AT,	BE,	CH,	DE.	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	Hυ,	SK	
IORITY	APP	LN.	INFO	. :					1	EP 2	002-	3801	20		A 2	0020	611
									1	EP 2	002-	3801	21		A 2	0020	611
											002-						

P 20021003 W 20030606 WO 2003-US15405

OTHER SOURCE(S): IT 635317-69-0P MARPAT 140:42463

635317-69-07
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of prodrugs of excitatory amino acids)
635317-69-0 CAPLUS
2-Thiabicyclo[3.1.0]hexane-4,6-dicarboxylic acid, 4-[[[(2S)-1-[(1,1-dimethylethoxylcarbonyl]-2-pyrrolidinyl]carbonyl]amino]-, dimethyl ester,
2,2-dioxide, (1R,4S,5S,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L10 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

JP 2005502703 T2 20050127 JP 2003-256882 20020909

US 2005014700 A1 20050120 US 2004-499006 20040827

PRIORITY APPLN. INFO:: US 2001-318179P P 20010909

WO 2002-US28749 W 20020909 OTHER SOURCE(S): MARPAT 138:255007

IT 372953-56-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
(aynthesis and evaluation of tetrahydrocyclopropa[c]benz[e]indol-4-one analogs of CC-1065 and the duocarmycins defining the contribution of the DNA-binding domain)
372953-56-5 CAPLUS
Carbamic acid, [5-[[[5-[[[18]-1-(chloromethyl)-1,2-dihydro-5-hydroxy-3H-benz[e]indol-3-yl]carbonyl]-3-thienyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

502171-77-9P

502171-77-99
RL: RCT (Reactant); SPN (Synthetic preparation); PREP [Preparation); RACT (Reactant or reagent)
(synthesis and evaluation of tetrahydrocyclopropa[c]benz[e]indol-4-one analogs of CC-1065 and the duocarmycins defining the contribution of the DNA-binding domain)
502171-77-9 CAPLUS
2-Thiophenecarboxylic acid, 4-[[[4-[[1,1-dimethylethoxy]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]- [9CI] (CA INDEX NAME)

ANSWER 6 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 21 Mar 2003

AB 132 CBI analogs I [X, Y = arylene, heteroarylene] of CC 1065 and the duocarmycins having dimeric monocyclic, bicyclic, and tricyclic heteroaroms. Substituents were synthesized by a parallel route. The resultant analogs were evaluated with respect to their catalytic and cytotoxic activities. The relative contribution of the various dimeric monocyclic, bicyclic, and tricyclic heteroaroms. Substituents within the DNA binding domain were characterized. Several of the resultant CBI analogs of CC 1065 and the duocarmycins were characterized as having enhanced catalytic and cytotoxic activities and were identified as having enhanced catalytic and cytotoxic activities and were identified as having attriting from 4-H2NC6H4CO2H and the hydrochloride salt of seco-CBI.

ACCESSION NUMBER: 2003:221652 CAPLUS

DOCUMENT NUMBER: 138:255007

TITLE: PREPARTATION OF CBI analogues of CC 1065 and the duocarmycins for therapeutic use as anticancer agents Boger, Dale L.

PATENT ASSIGNEE(S): The Scripps Research Institute, USA

CODEN: PIXKD2

DOCUMENT TYPE: Patent

LANGUAGE: English

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA:	TENT	NO.			KIN	D	DATE		- 1	APPL	ICAT	ION	NO.		D.	ATE	
						-									-		
WO	2003	0228	06		A2		2003	0320	1	WO 2	002-	US28	749		2	0020	909
WO	2003	0228	06		A3		2003	1113									
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		co,	CR,	cu,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,
		UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW							
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	52,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	ΚZ,	MD,	RU,	ΤJ,	TM,	AT,	BE,	BG,	CH,	CY,	cz,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	SK,	TR,	BF,	ВJ,	CF,
		CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG			
CA	2459	308			AA		2003	0320		CA 2	002-	2459	308		2	0020	909
EP	1423	110			A2		2004	0602	1	EP 2	002-	7982	01		2	0020	909
	R:	AT,	BE.	CH.	DE.	DK.	ES,	FR.	GB.	GR.	IT.	LI.	LU.	NL.	SE.	MC.	PT.

ANSWER 7 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 02 Jan 2003

AB Title compds. I (wherein R1 and R6 = independently H, halo, CF3, alkyl, alkylthio, alkoxy, CN, NO2, NH2, Ph, OPh, SPh, CH2Ph, OCH2Ph, SCH2Ph, or (un) substituted amido, carbamido, sulfonyl, etc.; R2 = H, halo, CF3, OH, alkyl, alkoxy, CHO, CN, NO2, (un) substituted amido, carbamido, sulfonyl, etc.; R2 = H, halo, CF3, OH, olly, olly, alkoxy, CHO, CN, NO2, (un) substituted amino, or alkylaulfonyl; R3 = CO2H, OPO3H2, SO3H, etc.; R4 = H, CF3, alkyl, alkoxy, (alkyl) cycloalkyl, etc.; and pharmaceutically acceptable salts thereof; were prepared as phospholipase enzyme inhibitors. For example, S-nitcoindole was C2-alkylated (551) with Me 4-(bromomethyl)-3-methoxybenzoate in dioxane, N-alkylated (571) with 1-iodopropane in a solution of TH7 and NaH, and converted to the amine (801) by hydrogenation using Pt/C. The amine was converted to the carbamate (391) by addition of cyclopentyl chloroformate in CH2C12 and 4-methylmorpholine, and the resultant ester was hydrolyzed to yield II (711). The latter inhibited cytosolic phospholipase A2 (CPLA2) by 501 at a concentration of 170 µN in a coumarin assay and reduced footpad volume by 16.61 at a dose of 5 mg/Kg IV in a carrageanan-induced footpad edema test on rats. Thus, I are useful for treatment of infilammatory conditions, such as arthritis, inflammatory bowel disease, and asthma (no data).

ACCESSION NUMBER: 2003:1275 CAPLUS
DOCUMENT NUMBER: 138:55866

Freparation of indole derivatives as phospholipase

Preparation of indole derivatives as phospholipase enzyme inhibitors for treatment of inflammatory conditions TITLE:

Seehra, Jasbir S.; McKew, John C.; Lovering, Frank; Bemis, Jean E.; Xiang, Yibin; Chen, Lihren; Knopf, INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

Genetics Institute, LLC, USA
U.S., 57 pp., Cont.-in-part of U. S. Ser. No. 256,062, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: LANGUAGE: English FAMILY ACC. NUM. COUNT:

PATENT NO. KIND DATE APPLICATION NO. DATE US 2000-686616 US 1998-113674P US 1999-256062 US 6500853 PRIORITY APPLN. INFO.: 20001011 B1 20021231

OTHER SOURCE(5): MARPAT 138:55866

IT 241497-74-5DP, 3-Thiophenecarboxylic acid, 4-{[[5[(cyclopentylcarbonyllamino]-1-(diphenylmethyl)-1H-indol-3yl]carbonyllamino]-, ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT RL: RCT (Reactant); SPN (Synthetic preparation); FRD: Irreparation; FND: (Reactant or reagent) (Intermediate; preparation of indole derivs. as phospholipase enzyme inhibitors for treatment of inflammatory conditions) 241497-74-5 CAPLUS 3-Thiophenecarboxylic acid, 4-[{[5-[(cyclopentylcarbonyl)amino]-1-(diphenylmethyl)-1H-indol-3-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

241497-74-5P, 3-Thiophenecarboxylic acid, 4-{{[5-[(cyclopentylcarbonyl)amino]-1-(diphenylmethyl)-1H-indol-3-yl]carbonyllamino]-RE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
 (phospholipase inhibitor; preparation of indole derivs. as phospholipase
 enzyme inhibitors for treatment of inflammatory conditions)
241497-74-5 CAPLUS
3-Thiophenecarboxylic acid, 4-[[[5-[(cyclopentylcarbonyl)amino]-1(diphenylmethyl)-1H-indol-3-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

RÉFERENCE COUNT:

THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 20 Dec 2002

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. I [Rl = H, F, Cl, CN, CF3, OH, N(R2)2, OR2, etc.; R2-3 = H, alkyl, heteroalkyl; n = 1-25; Y = alkylene, (hetero)aromatic; Z = O, N; m = 1 if Z = O, m = 2 if Z = N] were prepared For instance, II (preparation given)

Coupled to 4-chloro-2-fluorobenzoic acid, the product saponified and the resulting carboxylic acid coupled to N-(2-aminoethyl) morpholine to give III. III had MIC & 4 ug/ml. against B. cereus, E. feecalis, E. faecium, S. aureus, S. epidermidis and S. pneumoniae. A number of compds, of the invention were screened for their ability to bind to three DNA sites (binding data tabulated).

ACCESSION NUMBER: 2002:964476 CAPLUS
DOCUMENT NUMBER: 138:39101
TITLE: Preparation of antipathogenic poly-pyrrole-benzamide compounds

compounds
Burli, Roland W.; Kaizerman, Jacob A.; Jones, Peter
Genesoft, Inc., USA
PCT Int. Appl., 106 pp.
CODEN: PIXXD2
Patent
English

INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

LANGUAGE:		English			
FAMILY ACC. PATENT INFOR		4			
PATENT	NO.		E APPI	ICATION NO.	DATE

		A2 2002		:002-US17951	20020606
	101007	A3 2003			
W:					3Z, CA, CH, CN,
					SB, GD, GE, GH,
	GM, HR, HU,	ID, IL, IN,	, IS, JP, KE,	KG, KP, KR, F	KZ, LC, LK, LR,
					IO, NZ, OM, PH,
	PL, PT, RO,	RU, SD, SE,	, SG, SI, SK,	SL, TJ, TM, T	rn, TR, TT, TZ,
	UA, UG, US,	UZ, VN, YU,	, ZA, ZM, ZW		
RW:	GH, GM, KE,	LS, MW, MZ,	, SD, SL, S2,	TZ, UG, 2M, 2	W, AM, AZ, BY,
					ES, FI, FR, GB,
	GR, IE, IT,	LU, MC, NL,	, PT, SE, TR,	BF, BJ, CF, C	G, CI, CM, GA,
			, SN, TD, TG		
		A1 2003		002-165764	
PRIORITY APP	LN. INFO.:			001-298206P	
				001-342309P	P 20011221
OTHER SOURCE		MARPAT 138:	: 39101		
IT 478803-					
				nthetic prepar	
(Therap (Uses)	eutic use);	BIOL (Biolog	;ical study);	PREP (Prepara	tion); USES
	paration of DNA binders)	poly-pyrrole	-benzamide a	nd related and	logs as antibiotic
RN 478803-	58-6 CAPLUS				
CN 1H-Pyrr	ole-2-carbox	amide, 4-[[]	4-[(4-chlore	-2-fluorobenzo	yl)amino]-lH-
pyrrol-	2-yl]carbony	1]amino]-1-m	nethyl-N- (5- ([[2-[4-	-
morphol	inyl)ethyl]a:	mino] carbony	/1]-3-thienyl]- (9CI) (CA	INDEX NAME)

L10 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L10 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

ANSWER 9 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 09 Aug 2002

AB Title compds. [I; X = (substituted) (CH2)m; m = 1-3; R1 = (substituted) alkyl, alkenyl, alkynyl, aryl, heteroaryl, etc.; R2, R3 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R4, R41, R5, R51 = H, OH, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, alkoxy, etc.; R6, R61 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R7, R8 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R7, R8 = (substituted) (CR2)nH: n = 1-4; R7R8N = (substituted) dycloheteroalkyl), were prepared as cardiovascular agents (no data). 974 I, including (II), were prepared accession NUMBER: 2002:594840 CAPLUS
DOCUMENT NUMBER: 137:154858

TITLE:

INVENTOR (S):

137:154858
Preparation of arylsulfonamidopiperidones as inhibitors of Factor Xa. Stein, Philip P.; O'Connor, Stephen P.; Lawrence, R. Michael: Shi, Yan Bristol-Myers Squibb Company, USA PCT Int. Appl., 246 pp. CODEN: PIXXD2
Patent PATENT ASSIGNEE (S):

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	T NO.					DATE						NO.			ATE	
					-											
WO 20	020608	94		A2		2002	0808	1	NO 2	002-1	US25	42		2	0020	128
WO 20	020608	94		A3		2002	1219									
w	: AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
	co,	CR,	cu,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
	GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ŦJ,	TM,	TN,	TR,	TT,	TZ,
	UA,	UG,	US,	υz,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,
	TJ,	TM														
R	W: GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	υG,	ZM,	ZW,	ΑT,	BE,	CH,
	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE.	IT,	LU,	MC,	NL,	PT,	SE,	TR,
	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
CA 24	36774			AA		2002	8080		CA 2	002-	2436	774		2	0020	128
EP 13	58178			A2		2003	1105	1	EP 2	002-	7173	81		2	0020	128
R	: AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SĒ,	MC,	PT,
	IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR						
JF 20	045186	88		T2		2004	0624	,	JP 2	002-	5610	43		2	0020	128
US 65	55542			B1		2003	0429	1	US 2	002-	5962	1		2	0020	129
PRIORITY A	PPLN.	INFO.	. :					1	US 2	001-	2649	64P		P 2	0010	130

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 18 May 2002

AB The title compds. [I; X = O, S; Rl = CF3, CF2H, CFH2; R2 = alkyl, haloalkyl, alkoxyelkyl, haloalkoxyelkyl; R3 = H, Me, CF3, F; Q = substituted Ph, 2-thienyl, 3-thienyl] which have plant-protecting properties and are suitable for protecting plants against infestation by phytopathogenic microorganisms, were prepared Thus, treating I-methyl-4-trifluoromethylpyrrole-3-carboxylic acid with oxalyl chloride in the presence of a catalytic amount of DMF in CH2C12 followed by addition of the resulting acid chloride to a solution of 2-(1,3-dimethylbutyl)phenylamine and Et3N in CH2C12 afforded II. Compds. I showed good activity (< 20% infestation) against Puccinia recondita (brown rust) on wheat.

ACCESSION NUMBER: 2002:368451 CAPLUS
DOCUMENT NUMBER: 136:369602
Preparation of pyrrolecarboxamides - ---

136:369602
Preparation of pyrrolecarboxamides and pyrrolecarbothioanides as agrochemical fungicides Walter, Harald Syngenta Participations A.-G., Switz. PCT Int. Appl., 66 pp. CODEN: PIXXD2
Patent INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English

	TENT																
			~			-									-		
WO	2002	0385	42		A1		2002	0516	1	WO 2	001-	EP12	830		2	0011	106
	W:	AE,	AG.	AL.	AM.	AT.	ΑU,	AZ.	BA.	BB.	BG.	BR.	BY.	BZ.	CA.	CH.	CN.
							DK,										
		GM.	HR.	HU.	ID.	IL.	IN,	IS.	JP.	KE.	KG.	KP.	KR.	KZ.	LC.	LK.	LR.
							MD,										
							SG,										
							ZW,										
	RW:	GH,															
		DΕ,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		BJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
CA	2426	033			AA		2002	0516		CA 2	001-	2426	033		2	0011	106
ΑU	2002	0236	68		A5		2002	0521		AU 2	002-	2366	8		2	0011	106
EP	1341	757			A1		2003	0910		EP 2	001-	9935	99		2	0011	106
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE.	SI.	LT.	LV.	FI.	RO,	MK,	CY,	AL.	TR						
BR	2001	0152	00		A		2004	0217		BR 2	001-	1520	0		2	0011	106
EG	2312	2			A		2004	0428		EG 2	001-	1173			2	0011	106
.10	2004	5121	67		772		2004	0430		10 2	002-	5410	70			0011	106
	2005																
US	∠005	11791	30		Al		2005	0002		us Z	UU3-	4195	13		2	0011	TAP

Page 2630/08/2005

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L10 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
WO 2002-US2542 W 20020128
OTHER SOURCE(S): MARPAT 137:154858
IT 445277-00-99
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
            (Uses)
(preparation of arylsulfonamidopiperidones as inhibitors of Factor Xa)
445277-00-9 CAPLUS
2-Pyrrolidinecarboxamide, 1-[[(3S)-3-[[[(1E)-2-(5-chloro-2-thienyl]sulfonyl]amino]-2-oxo-1-piperidinyl]acetyl]-N-(tetrahydro-1,1-dioxido-3-thienyl)-, (2S)- (9CI) (CA INDEX NAME)
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Absolute stereochemistry.
Double bond geometry as shown.

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L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS ON STN ZA 2003003012 A 20040520 ZA 2003-3012 GB 2000-27284 GB 2000-30268
                                                                                                                                                                                                                                                                                  (Continued)
                                                                                                                                                                                                                                                                                                                 20030416
                                                                                                                                                                                                                                                                                                   A 20001108
A 20001212
W 20011106
                                                                                                                                                                                                                                                                                                                20001212
                    R SOURCE (S): MARPAT 136:369602
424832-40-6P 424832-41-7P 424832-42-8P
424832-43-9P 424832-44-0P 424832-45-1P
424832-45-2P 424832-44-0P 424832-45-1P
424832-45-2P 424832-50-8P 424832-51-9P
424832-55-3P 424832-53-1P 424832-55-3P
424832-55-3P 424832-53-1P 424832-55-5P
424832-55-8P 424832-56-4P 424832-55-5P
424832-65-6P 424832-65-9P 424832-65-9P
424832-61-1P 424832-65-5P 424832-65-9P
424832-67-7P 424832-67-9P 424832-67-P
424832-79-P 424832-71-3P 424832-73-P
424832-79-P 424832-71-3P 424832-73-P
424832-79-P 424832-71-3P 424832-73-P
424832-79-P 424832-71-3P 424832-75-P
424832-79-P 424832-71-3P 424832-78-P
424832-79-P 424832-71-3P 424832-81-8P
RL: AGR (Agricultural use): SSU (Slolo
 OTHER SOURCE(S):
                        RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
                      (Uses)
(preparation of pyrrolecarboxamides and pyrrolecarbothioamides as agrochem. fungicides)
424832-40-6 CAPLUS
H-Pyrrole-3-carboxamide, N-[2-{1,3-dimethylbutyl}-3-thienyl}-1-methyl-4-(trifluoromethyl)- {9CI} (CA INDEX NAME)
```

424832-41-7 CAPLUS IH-Pyrcole-3-carboxamide, N-[2-(1,3-dimethylbutyl)-3-thienyl]-1-(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

424832-42-8 CAPLUS
IH-Pyrrole-3-carboxamide, 1-methyl-N-[2-(3-methyl-1-(trifluoromethyl)butyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CF3 1-Bu-CH 0 1-NH-CH NH-CH

RN 424832-43-9 CAPLUS
CN 1H-Pyrrole-3-carboxamide, l-methyl-4-(trifluoromethyl)-N-[2-[4,4,4-trifluoro-1-methyl-3-(trifluoromethyl)butyl]-3-thienyl]- (9CI) (CA INDEX NAMF)

RN 424832-44-0 CAPLUS
CN HH-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylpentyl)-3-thienyl]-1-methyl-4(trifluoromethyl)- (SCI) (CA INDEX NAME)

RN 424832-45-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylpentyl)-3-thienyl]-1(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Et₂CH-CH₂-CH

RN 424832-49-5 CAPLUS
CN 1H-Pyrcle-3-carboxamide, N-[2-(1,3-dimethylbutyl)-3-thienyl]-2-fluoro-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 424932-50-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylbutyl)-3-thienyl}-2-fluoro-1(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 424832-51-9 CAPLUS
CN IN-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylpentyl)-3-thienyl]-2-fluoro-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me | He | CF3

RN 424832-52-0 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1-methyl-N-[2-{3-methyl-1-

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 424832-46-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylbutyl)-5-fluoro-3-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me CH-Bu-i

RN 424832-47-3 CAPLUS
CN lH-Pyrrole-3-carboxamide, N-{2-(1,3-dimethylbutyl)-4-fluoro-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me CH-Bu-i

RN 424832-48-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(3-ethyl-1-methylpentyl)-3-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (trifluoromethyl)butyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

CF3 1-Bu-CH O CF3

RN 424832-53-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1-methyl-N-[2-[3-methyl-1-(trifluoromethyl)pentyl]-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me | CF3 | CF3 | CF3 | CF3 | CF3 | MH - C | MH -

RN 424832-54-2 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[2-(1,3-dimethylbutyl)-3-thienyl]-1-methyl- (9Cl) (CA INDEX NAME)

i-Bu-CH NH-C

RN 424832-55-3 CAPLUS
CN H-Pyrcole3-carboxamide, 4-(difluoromethyl)-N-[2-(1,3-dimethylpentyl)-3-thienyl]-1-methyl (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

424832-56-4 CAPLUS 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-{2-{3-methyl-1-(trifluoromethyl)butyl}-3-thienyl}- (9CI) (CA INDEX NAME)

424832-57-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1,3-dimethylbutyl)-3-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

424832-58-6 CAPLUS 1H-Pyrrole-3-carboxamide, N-{2-(1,3-dimethylpentyl)-3-thienyl}-4-(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

424832-62-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(lR,25,4R)-bicyclo[2.2.1]hept-5-en-2-yl-3-thienyl]-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

424832-63-3 CAPLUS
IH-Pyrrole-3-carboxamide, N-{2-{IR,2R,4S}-bicyclo{2.2.1}hept-2-yl-3-thlenyl-}-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

424832-59-7 CAPLUS
1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-{2-[3-methyl-1-(trifluoromethyl)butyl}-3-thienyl}- (9CI) (CA INDEX NAME)

424832-60-0 CAPLUS
IN-Pyrole-3-carboxamide, N-{2-bicyclo[2.2.1]hepta-2,5-dien-2-y1-3-thienyl)-1-methyl-4-{trifluoromethyl)- (9CI) (CA INDEX NAME)

424832-61-1 CAPLUS 1M-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.1]hept-2-en-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

424832-65-5 CAPLUS
1H-Pytrole-3-carboxamide, 1-methyl-4-(trifluoromethyl)-N-[2-[(1R,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl]-3-thienyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

424832-66-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-1-(methoxymethyl)-4-(trifluoromethyl)-, rel- [9CI] (CA INDEX

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

424832-67-7 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4s)-bicyclo[2.2.1]hept-2-yl-3-thienyl]-4-(difluoromethyl)-1-methyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

424832-68-8 CAPLUS 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]octa-2,5-dien-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

424832-71-3 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-bicyclo(2.2.2)oct-2-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

424832-72-4 CAPLUS | H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-1-(methoxymethyl)-4-(trifluoromethyl)- (9Cl) (CA INDEX NAME)

424832-73-5 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-4-fluoro-3-thienyl)1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

424832-69-9 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-bicyclo{2.2.2}oct-2-en-2-yl-3-thlenyl}-1-methyl-4-{trifluoromethyl}- (9CI) (CA INDEX NAME)

424832-70-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-(1R,2S,4R}-bicyclo[2.2.2}oct-5-en-2-yl-3-thienyl}-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 424832-74-6 CAPLUS
CN | H-Fyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-4-fluoro-3-thienyl)|-(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

424832-75-7 CAPLUS
1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

424832-76-8 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.1]hept-5-en-2-yl-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 424832-77-9 CAPLUS

(N 1H-Pyrrole-3-carboxamide, N-{2-(1R,2R,4S}-bicyclo[2.2.1]hept-2-yl-3-thienyl}-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry

RN 424832-78-0 CAPLUS

RN-Pyrrole-3-carboxamide, N-{2-(1R,2S,4R)-bicyclo{2.2.1}hept-5-en-2-yl-3-thienyl]-2-fluoro-1-(methoxymethyl)-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continue

RN 424832-81-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo(2.2.2)oct-2-yl-3-thienyl)-2-fluoro1-methyl-4-(trifluoromethyl)- (SCI) (CA INDEX NAME)

RN 424832-82-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-2-fluoro1-(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 424832-83-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2R,4S)-bicyclo[2.2.1]hept-2-yl-3-thienyl}-1,2-dimethyl-4-(trifluoromethyl)-, rel- [9CI] (CA INDEX NAME)

Page 3030/08/2005

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 424832-79-1 CAPLUS
CN HH-Pyrrole-3-carboxamide, N-[2-{1R,2R,4S}-bicyclo[2.2.1}hept-2-yl-3-thienyl]-2-fluoro-1-(methoxymethyl)-4-{trifluoromethyl}-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 424832-80-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[2-(1R,2S,4R)-bicyclo[2.2.2]oct-5-en-2-yl-3-thienyl]-2-fluoro-1-methyl-4-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
Relative stereochemistry.

RN 424832-84-8 CAPLUS
CN 1H-Pytrole-3-carboxamide, N-(2-bicyclo[2.2.2]oct-2-yl-3-thienyl)-1,2-dimethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 21 Dec 2001

The development of a solution-phase synthesis of distamycin A and its extension to the preparation of 2640 analogs are described. Thus,

extension to the preparation of 2640 analogs are described. Thus, solution-phase synthesis techniques with reaction workup and purification employing acid/base liquid-liquid extns. were used in the multistep preparation of distanycin A (8 steps, 40 overall yield) and a prototypical library of 2640 analogs providing intermediates and final products that are ≥ 95 pure on conventional reaction scales. Screening the prototypical library provided compds. that are 1000 times more potent than distanycin A in cytotoxic assays (1, Boc = tert-butoxycarbonyl, ICSO = 29 nM, IJ210), that bind to poly(dA)-poly(dT) with comparable affinity, and that exhibit an altered DNA binding sequence selectivity. Several candidates were identified which bound the five base-pair AT-rich site of the PSA-ARE-3 sequence, and one (II, R = 4-dimethylaminobutyryl; K = 3.2 x 106 M-1) maintained the high affinity binding (K = 4.5 x 106 M-1) to the ARE-consensus sequence containing a GC base-pair interrupted five base-pair rat-rich site suitable for inhibition of gene transcription initiated by hormone insensitive androgen receptor dimerization and DNA binding characteristic of therapeutic resistant prostate cancer.

ACCESSION NUMBER: 2001:923774 CAPLUS

2001:923774 CAPLUS 136:54024 ACCESSION NUMBER: DOCUMENT NUMBER:

Preparation of distamycin A analogs and screening for DNA binding and cytotoxic activities TITLE:

L10 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Boger, Dale L. Scripps Research Institute, USA PCT Int. Appl., 93 pp. CODEN: PIXXD2 INVENTOR(S): PATENT ASSIGNEE(S): DOCUMENT TYPE: Patent FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 2001096313 Al 20011220 WO 2001-US19404 20010614

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FT, GB, GD, GE, H, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, IV, MA, MD, MG, MK, NH, MM, WK, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SC, TR, BF, BJ, CF, CG, CI, CM, GA, GM, GW, ML, MR, NE, SM, TD, TG

PRIORITY APPLN. INFO: US 2000-211760P P 20000614

OTHER SOURCE(S):

TH 292069-27-3P 292069-37-SP

RL: CPN (Combinatorial preparation): PAC (Pharmacological activities). MU 20010614 WO 2001096313 20011220 WO 2001-US19404 A1

292069-27-3P 292069-37-5P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU
(Therapeutic use); BIOL (Biological atudy); CMBI (Combinatorial study);
PREP (Preparation); USES (Uses)
(preparation of distamyoin A analogs and screening for DNA binding and
cytotoxic activities)
292069-27-3 CAPLUS
Benzo(1, 2-b:4, 3-b'|dipyrrole-2-carboxylic acid, 6-[[4-[[[4-[(1,1-dimethylethoxylcarbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-2thienyl]carbonyl]-3,6,7,8-tetrahydro-, methyl ester (9CI) (CA INDEX NAME)

292069-37-5 CAPLUS

Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-[[4-[[4-[[4-(dimethylamino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-2-thlenyl]carbonyl]-3,6,7,8-tetrahydro-, methyl ester (9CI) (CA INDEX

LIO ANSWER 12 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 12 Oct 2001

AB Charged compds. are provided that have one or more regions of localized pos. charge, as are compns. comprising such compds., methods of synthesizing such compds. methods of screening such compds. to identify those having anti-infective activity, and methods of using such compds. to prevent or inhibit infections. These compds., and compns. containing them, have multiple applications, including use in human and animal medicine and in agriculture.

ACCESSION NUMBER: 2001:747848 CAPLUS

135:298753

DOCUMENT NUMBER: 135:298753
Charged compounds having a nucleic acid-binding moiety, their preparation, and their use as antilifective agents
Ge, Yigong; Taylor, Matthew J.; Baird, Eldon E.; Moser, Heinz E.; Burli, Roland W.
Genesoft, Inc. USA
PCT Int. Appl. 62 pp.
CODEN: PIXXD2
Patent
FERSITED

INVENTOR (S):

PATENT ASSIGNEE (S):

SOURCE:

DOCUMENT TYPE: LANGUAGE:

English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE A2 A3 20011011 WO 2001074898 WO 2001-US8252 20010314 2010174898 A3 20030116
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BB, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, NN, MM, MX, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FIT, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GM, ML, MR, NE, SN, TD, TG
2403537 AA 20011011 CA 2001-2403537 20010314
26052693 A2 20030429
2603529609 TZ 20031007 JP 2001-572587 20010314
26595691 A1 20021216 EP 2001-594573 20010314
265921 A1 20021216 EP 2001-594573 20010314 WO 2001074898 CA 2403537 US 2002065227 US 6555693 US 6555693 B2 20030429
JP 2003529609 T2 20031007 JP 2001-572587 20010314
EP 1265921 A1 20021218 EP 2001-954573 20010316
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LW, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
US 2003211508 A1 20031113 US 2002-278870 20021022
RITY APPLN. INFO::
US 2001-808729 A2 20010314
WG 2001-808729 A3 20010314 20021022 P 20000316 A3 20010314 W 20010314 PRIORITY APPLN. INFO.: WO 2001-US8252

MARPAT 135:298753 OTHER SOURCE(S): IT 365211-00-3

RE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(charged compds. with nucleic acid-binding moiety, preparation, and use as

(charged compds. With nucleic acid-binding moiety, preparation, and use a antiinfective agents)
365211-00-3 CAPLUS
3-Isothiazolecarboxamide, 4-chloro-5-[[3-(dimethylamino)propyl]amino]-N-[5-[[[3-(dimethylamino)propyl]amino]carbonyl]-3-thienyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-(CA INDEX NAME)

L10 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

PAGE 1-A

L10 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2005 ACS on STM (Continued)
REFERENCE COUNT: 1 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 13 Sep 2001

AB The solution-phase, parallel synthesis and evaluation of a library of 132 (+)-1,2,9,9-tetrahydrocycloprops[c]benz[e]indol-4-one (CBI) analogs of CC-1065 and the duocarmycins containing dimeric monocyclic, bicyclic, and tricyclic heteroarom replacements for the DNA-binding domain are described. This systematic study revealed clear trends in the structural requirements for observation of potent cytotoxic activity and DNA alkylation efficiency, the range of which spans a magnitude of 210 000-fold. Combined with related studies, these results highlight that the role of the DNA-binding domain goes beyond simply providing DNA-binding selectivity and affinity (10-100-fold enhancement in properties), consistent with the proposal that it contributions simply providing DNA-binding selectivity and affinity (10-100-fold enhancement in properties), consistent with the proposal that it contributions simply providing DNA-binding of admin 1000-fold enhancement in properties).

ACCESSION NUMBER: 2001:667407 CAPLUS
DOCUMENT NUMBER: 2001:667407 CAPLUS
DOCUMENT NUMBER: 2001:667407 CAPLUS

TITLE: Parallel Synthesis and Evaluation of 132 (+)-1,2,9,9a-Tetrahydrocyclopropa[c]benz[e].indol-4-one (CBI) Analogues of CC-1065 and the Duocarmycins Defining the Contribution of the DNA-Binding Domain Boger, Dale L.: Schmitt, Harald W.: Fink, Brian E.: Hedrick, Michael P.

PEPARTMENT OF A STATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA

Journal of Organic Chemistry (2001), 66(20), 6654-6661 CODEN: JOCEAU: ISSN: 0022-3263

American Chemical Society
Journal LINGUAGE: English

COTHER SOURCE(S): TATASSA-54-54 English CASREACT 135:357786 OTHER SOURCE(S): IT 372953-56-5P 372933-56-59
RL: ADV (Adverse effect, including toxicity): BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation) (synthesis and evaluation of tetrahydrocyclopropa(c)benz[e]indol-4-one analogs of CC-1065 and the duocarmycins defining the contribution of the DNA-binding domain)
372933-56-5 CAPLUS
Carbamic acid, (5-[[[5-[[(1S)-1-(chloromethyl)-1,2-dihydro-5-hydroxy-3H-benz[e]indol-3-yl]carbonyl]-3-thienyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yll-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 27 Jul 2001 GI

AB The title compds. [I: X = O, S: Rl = alkyl, cycloalkyl, halo: R2 = H, alkyl, alkoxy, etc.: R3 = alkyl; A = (un)substituted ortho-substituted (hetero)aryl, bicyclo(hetero)aryl) which have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms, were prepared Thus, methylation of Me 4-methylpyrrole-3-carboxylate followed by hydrolysis of the resulting ester, and reaction of 1,4-dimethylpyrrole-3-carboxylic acid with 2-(4'-fluorophenyllanillan afforded I [X = O; Rl, R3 = Me: R2 = H; A = 4'-fluorobiphenyl-2-yl] which showed strong efficacy against Puccinia recondita on wheat (< 200 infestation).

ACCESSION NUMBER: 135:137397

TITLE: Preparation of pyrrolecarboxamides and pyrrolethioamides as fungicides

INVENTOR(S): Syngenta Participations A.-G., Switz.

POT Int. Appl., 111 pp.

DOCUMENT TYPE: PIXXD2

POCUMENT TYPE: Patent

LANGUAGE: Patent English FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WC 2001053259 Al 20010726 WC 2001-EP592 Z0010119

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CR, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LM, LV, LV, MA, MD, MG, MK, MM, MM, KK, MZ, NO, MZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VU, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, ML, PT, SE, TR, BF, BJ, CF, CG, CI, CH, GA, GR, GW, ML, MR, RS, SN, TD, Z0010119

BR 2001007738 A 20010726 CA 2001-2397008 20010119

BR 2001007738 A 20021025 BR 2001-7738 20010119

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2003520269 T2 20030762 JP 2001-503263 20010119

AL 702005641 A 20031103 CA 2002-181702 20021008

US 6806286 B2 200401019 PATENT NO.

L10 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN US 2004106521 A1 20040603 US 2003-680346 GB 2000-1447 GB 2000-1447 W0 2001-EP592 US 2002-181702 (Continued) 20031007 A 20000121 W 20010119 OTHER SOURCE(S): MARPAT 135:137397

IT 351416-74-5P 351416-75-6P 351416-76-7P

R1: AGR (Agricultural use): BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation): USES (Uses) (preparation of pyrrolecarboxamides and pyrrolethioamides as fungicides)

RN 351416-74-5 CAPLUS HH-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl)-1.4-dimethyl-(9CI) (CA INDEX NAME)

351416-75-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-4-(pentafluoroethyl)- (SCI) (CA INDEX NAME)

351416-76-7 CAPLUS 1H-Pyrrole-3-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 13 Jul 2001 $_{\rm GI}$

AB The title compds. [I; X = 0, S; Rl = H, alkyl, halo; R2 = alkyl; A = ortho-substituted aryl, ortho-substituted heteroaryl, bicycloaryl, bicycloheteroaryl] which have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms, were prepared E.g., a multi-step synthesis of I [Rl = H; R2 = Me; X = 0; A = 4-(4-chlorophenyl)pyridin-3-yl] which showed strong efficacy against Erypsiphe graminis on barley, was given.

ACCESSION NUMBER: 2001:507677 CAPLUS
DOCUMENT NUMBER: 135:92539

TITLE: reparation of trifluoromethylpyrole carboxamides and trifluoromethylpyrolebioamides are fundicides.

135:92539
Preparation of trifluoromethylpyrrole carboxamides and trifluoromethylpyrrolethioamides as fungicides Walter, Harald; Trah, Stephan; Schneider, Hermann Syngenta Participations A.-G., Switz.
PCT Int. Appl., 65 pp.
CODEN: PIXXD2
Patent INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE: English FAMILY ACC. NUM. COUNT:

TE	NT :	INFOR	MATI	ON:														
												LICAT						
	WO											2000-						
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			CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES.	, FI,	GB,	GD,	GE,	GH,	GM,	HR,
			ΗU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP.	, KR,	KZ,	LC,	LK,	LR,	LS,	LT,
			LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX.	, MZ,	NO,	NZ,	PL,	PT,	RO,	RU,
			SD,	SE,	5G,	SI,	sĸ,	SL,	TJ,	TM,	TR.	, TT,	TZ,	UA,	UG,	US,	UZ,	VN,
			YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KŻ,	MD	, RU,	TJ,	TM				
		RW:	GH,	GM,	KE,	LS,	MW.	MZ,	SD,	SL,	SZ	. TZ.	UG.	ZW.	AT,	BE.	CH.	CY.
			DE.	DK,	ES.	FI,	FR.	GB,	GR,	IE,	IT	LU,	MC.	NL.	PT.	SE.	TR.	BF,
												MR.						
	ÇA	2395	267			AA		2001	0712		CA	2000-	2395	267		2	0001	111
	BR	2000	0168	71		A		2002	1008		BR :	2000-	1687	1		2	0001	111
	ΕP	1252	139			A1		2002	1030		EP :	2000~	9850	16		2	0001	111
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			IE.	SI.	LT.	LV.	FI.	RO.	MK.	CY.	AL.	. TR						
	JP	2003	5192	12		T2		2003	0617		JP :	2001-	5502	04		2	0001	111
	EG	2259	9			Ā		2003	0430		EG :	2000-	1588			2	0001	224
	ZA	2002	0048	74		A		2003	0918		ZA :	2001- 2000- 2002-	4874			2	0020	618
	US	6699	818			B1		2004	0302		US	2002-	1692	R1		- 5	0021	008
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L10 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN OTHER SOURCE(S): MARPAT 135:92539 IT 349466-95-9P 349486-96-OP 349486-97-1P 349465-98-2P (Continued)

349486-98-2P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of trifluoromethylpyrrole carboxamides and trifluoromethylpyrrolethioamides as fungicides)
349486-95-9 CAPLUS

H-Pyrrole-3-carboxamide, 1-methyl-N-[2-(4-methylcyclohexyl)-3-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

349486-96-0 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(4-isoxazoly1)-3-thieny1)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

349486-97-1 CAPLUS
1H-Pyrcole-3-carboxamide, N-{2-(3-fluoro-4-pyridinyl)-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

349486-98-2 CAPLUS
1H-Pyrrole-3-carboxamide, N-{2-{1,2-dihydro-2-oxo-3-pyridinyl}-3-thienyl}-1-methyl-4-{trifluoromethyl}- (9CI) (CA INDEX NAME)

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,

CG, CI, CM, GA, GM, GM, ML, MR, NE, SN, TD, TG

BR 2000008105 A 20001810 CA 2000-2355734 20000131

EP 1173421 A2 20020123 EP 2000-901747 20000131

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO

JP 2002536362 T2 20020123 JP 2000-597270 2000131

NO 2001003176 A 20011001 NO 2001-3768 20016619

NO 20031360 B1 20041221 US 2001-809516 20011002

PRIORITTY APPLN. INFO::

GB 1999-2455 A 19990205

PROORITTY APPLN. INFO::

GB 1999-2455 A 199902013 JP 2000-597270
ZA 2001-5017
NO 2001-3768
US 2001-889516
GB 1999-2455
WO 2000-GB284

OTHER SOURCE(s): MARPAT 133:150463

IT 287725-88-6P

RI: BAC [Biological activity or effector, except adverse); BSU (Biological study, unclassified); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis)

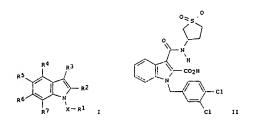
RN 287725-88-6 CAPIUS

CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl)-3-[((tetrahydro-1,1-dioxido-3-thienyl)amino)carbonyl)- (9CI) (CA INDEX NAME)

287726-47-0P

287726-47-09
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis)
287726-47-0 CAPLUS
1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3[(tetrahydro-1,1-dioxido-3-thienyl)amino]carbonyl]-, ethyl ester (9CI)
(CA INDEX NAME)

ANSWER 16 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 11 Aug 2000



AB The title compds. [1; X = CH2, SO2; R1 = (un)substituted aryl, heteroaryl; R2 = CO2H, CN, COCH2OH, etc.; R3 = OR15 (wherein R15 = substituted alkyl or cycloalkyl, (un)substituted heteroaryl), S(O)qR15 (q = O-2), (CR2)aCO2H (s = O-4), etc.; R4-R7 = H, (un)substituted hydrocarbyl, heterocyclyl, etc.) and their pharmaceutically acceptable salts, amides or esters, useful in the preparation of a medicament for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemoatxis, were prepared and formulated. Thus, hydrolysis of the corresponding ester afforded 93% II which showed 1C50 of 6.86 µM against hMCP-1 receptor binding. ACCESSION NUMBER: 2000:553556 CAPLUS 2000:UMENT NUMBER: 133:150463 Preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemoattractant protein-1 and/or RANTES induced chemoatxis Pauli, Alan Wellington; Kettle, Jason Astrazeneca UK Limited, UK PCT Int. Appl., 72 pp. CODEN: PIXXD2 PATENT TYPE: EARGUAGE: English PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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WO	2000	0461	99		A2		2000	0810	1	WO 2	000-0	GB28	4		2	0000	131
WO	2000	0461	99		A3		2000	1130									
	W:	ΑE,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU
		CZ,	DÉ,	DK,	DM,	ĒΕ,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL
		IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA
		MD,	MG,	MK,	MN,	MW,	MX,	NO,	NŻ,	PL,	PT,	RO,	Ŕυ,	SD,	SE,	SG,	SI
		SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZW,	AM
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM								
	RW:	GH.	GM.	KE.	LS.	MW.	SD,	SL.	SZ.	TZ.	UG.	ZW.	AT.	BE.	CH.	CY.	DE

L10 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 17 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 20 Jun 2000

The development of a solution-phase synthesis of distamycin A and its extension to the preparation of 2640 analogs are described. Thus, $\frac{1}{2} \left(\frac{1}{2} \right) \left(\frac{1}{2$

AB The development of a solution-phase synthesis of distamycin A and its extension to the preparation of 2640 analogs are described. Thus, solution-phase synthesis techniques with reaction workup and purification employing acid/base liquid-liquid extns. were used in the multistep preparation of distamycin A (8 steps, 40% overall yield) and a prototypical library of 2640 analogs providing intermediates and final products that are 25% pure on conventional reaction scales. The complementary development of a simple, rapid, and high-throughput screen for DNA binding affinity based on the loss of fluorescence derived from displacement of prebound ethidium bromide is disclosed which is applicable for assessing relative or absolute binding affinity to DNA homopolymers or specific sequences (hairpin oligonucleotides). Using hairpin oligonucleotides, this method permits the screening of a library of compds. against a single predefined sequence to identify high affinity binders, or the screening of a single compound against a full library of individual hairpin oligonucleotides to define its sequence selectivity. The combination permits the establishment of the complete DNA binding profile of each member of a library of compds. Screening the prototypical library provided compds. that are 1000 times more potent than distamycin A in cytotoxic assays [1, Boc = tert-butoxycarbonyl: [CSO = 29 nM, Ll210), that bind to poly[dA]-poly[dT] with comparable affinity, and that exhibit an altered DNA binding sequence selectivity. Several candidates were identified which bound the

L10 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(dimethylamino)-1-oxobutyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]2-thienyl]carbonyl]-3,6,7,8-tetrahydro-, methyl ester (9CI) (CA INDEX

292070-05-4P 292071-72-8P

292070-05-49 292071-72-89 RE: RCT (Reactant); PREP (Preparation); RACT (Reactant) SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (total synthesis of distamycin A and solution-phase combinatorial approach to distamycin A analogs as DNA binding agents)
2-Thiophenecarboxylic acid, 4-[([4-[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-lH-pyrrol-2-yl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

292071-72-8 CAPLUS
2-Thiophenecarboxylic acid, 4-[[[4-[[[4-[[[1,1-dimethyle-thoxy]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-2-thienyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

L10 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
five-base-pair AT-rich site of the PSA-ARE-3 sequence, and one (II, R =
4-dimethylaminobutyryl; K = 3.2 + 106 M-1) maintained the high
affinity binding (K = 4.5 + 106 M-1) to the ARE-consensus sequence
contg. a GC base-pair interrupted five-base-pair AT-rich site suitable for
inhibition of gene transcription initiated by hormone insensitive androgen
receptor dimerization and DNA binding characteristic of therapeutic
resistant prostate cancer.

ACCESSION NUMBER: 2000:495663 CAPLUS
DOCUMENT NUMBER: 133:223039
TOTAL Synthesis of Distamycin A and 2640 Analogs: A
Solution-Phase Combinatorial Approach to the Discovery
of New, Bioactive DNA Binding Agents and Development
of a Rapid, High-Throughput Screen for Determining
Relative DNA Binding Affinity or DNA Binding Sequence
Selectivity

of a Rapid, High-Throughput Screen for Determining
Relative DNA Binding Affinity or DNA Binding Sequence
Selectivity

BOGET, Dale L.: Fink, Brian E.: Hedrick, Michael P.

CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La
Jolla. CA, 92037, USA

SOURCE: Journal of the American Chemical Society (2000),
122(27), 6392-6394
CODEN: JACSART, ISSN: 0002-7863

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
COTHER SOURCE(S): CASREACT 133:223039

IT 220059-27-3P 292069-37-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified): SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
((cotal synthesis of distamycin A and solution-phase combinatorial approach to distamycin A analogs as DNA binding agents)

RN 292069-27-3 CAPIUS

CN Benzo(1, 2-b: 4, 3-b') idipyrrole-2-carboxylic acid, 6-[[4-[[[4-[[(1,1-dimethyl=thexy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-2-thienyl]carbonyl]-3, 6, 7, 8-tetrahydro-, methyl ester (9CI) (CA INDEX NAME)

292069-37-5 CAPLUS

Benzo[1,2-b:4,3-b']dipyrrole-2-carboxylic acid, 6-[[4-[[[4-[[4-

L10 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 18 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 25 Feb 2000

Title compds. I (R1 = H, halo, alkyl, haloalkyl; R2 = alkyl, haloalkyl, alkoxyalkyl, cyano, alkylsulfonyl, arylsulfonyl, etc.: A = substituted Ph, substituted 3-thienyl, substituted 4-indanyl) were prepared as plant protectants. Thus, 1.9 g l-methyl-4-(trifluoromethyl)pyrrole-3-carboxylic acid, obtained from Et 4,4-trifluorocrotonate, tosylmethyl isocyanide, and MeI, and 0.9 mL oxalyl chloride in 20 mL CH2C12 was stirred at room temperature in the presence of a catalytic amount of DMF, the solvent was orated

temperature in the presence of a catalytic amount of DMF, the solvent was evaporated under reduced pressure to give a crystalline solid, and the solid was added to a solution of 1.7 g of 2-biphenylamine and 4.2 mL Et3N in 20 mL CH2C12 at 0°, and the reaction mixture was stirred for 2 h at room temperature to give I (R1 = H, R2 = He, A = 2-biphenylyl). Application of this compound on apples, grapes, and tomatoes resulted in <10% infestation by Botrytis cinera.

ACCESSION NUMBER: 2000:133660 CAPLUS TOTAL AND THE SOLUTION OF THE

2000009482 A1 200000224 W0 1999-EP5837 19990810
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LK, LS, LT, LU, LV, MD, MG, MK, MN, MW, MN, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TH, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CT, CM, GA, GN, GW, ML, MR, NE, SN, TD, TS, BF, BJ, CF, CG, TS6831 B 20000306 AU 1999-58107745 19990810
9912962 A 20010508 BR 1999-19627 19990810 WO 2000009482 CI, TW 576831 AU 9955138 AU 756140 BR 9912962 BR 1999-12962 EP 1999-941573 20010613 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

L10 ANSWER 18 OF 22 . CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2005 ACS ON STN

IE, SI, LT, LV, FI, RO

TR 200100478 T2 20010621 TR 2001-2001

JP 2002522526 T2 20020723 JP 2000-5649

US 2002019541 A1 20020214 US 2001-7808

US 6365620 B2 20020402 (Continued) TR 2001-200100478 JP 2000-564936 US 2001-780897 20010209 PRIORITY APPLN. INFO.: GB 1998-17548 WO 1999-EP5837 19980812 19990810

except adverse); BSU (Biological

258510-89-3 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl}-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

CAPLUS

HP-Pyrrole-3-carboxamide, N-(2-[1,1'-biphenyl]-4-yl-3-thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

ANSWER 19 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 08 Sep 1999

AB Indole derivs. (I) and (II) [where R1 = H, halogen, CF3, C1-10 alkyl, S-C1-10 alkyl, C1-10 alkoxy, CN, NO2, NN2, Ph, OPh, SPh, CH2Ph, OCH2Ph, SCH2Ph, or (un) substituted amido, carbamido, sulfonyl, etc.; R2 = H, halogen, CF3, OH, C1-10 alkyl, C1-10 alkoxy, CHO, CN, NO2, (un) substituted amino, SO2-C1-6 alkyl; R3 = (un) substituted carboxylic acid, OPO3H2, SO3H, etc.; R4 = H, CF3, C1-6 alkyl, C1-6 alkoxy, (C1-6 alkyl)cycloalkyl, CHO, halogen, etc.; R5 = C1-6 alkyl, C1-6 alkoxy, (C1-6 alkyl)cycloalkyl, etc.] and pharmaceutically acceptable salts thereof, were prepared by several methods. Thus, 5-nitroindole was C3-alkylated with Me 4-(bromomethyl-3-methoxybenzoate in dioxane, N-alkylated with 1-iodopropane in a solution of THF and NaH, and converted to the amine by hydrogenation over Pt/C. The amine was converted to the amine by addition of cyclopentyl chloroformate in CH2C12 and 4-methylmorpholine and the resultant ester hydrolyzed to yield 4-(5-[(cyclopentyloxylcarbonyl]amino)-1-propyl-1H-indol-3-yl)methyl]-3-methoxybenzoic acid (III). The title compds are useful as phospholipase enzyme inhibitors, especially cytosolic phospholipase A2 (cPLAZ), for treatment of inflammatory conditions, particularly where inhibition of production of prostaglandins, leukotrienes, and PAF are all desired. Over one hundred compds of the invention were tested for cPLA2 inhibiting activity in the Coumarine assay and rat carragenan-induced footpad edema test. Compds. exhibited 7% to 98% inhibition at concns. of 0.125 µM to 400 µM in the footpad edema test.

ACCESSION NUMBER: 1399:566026 CAPLUS
DOCUMENT NUMBER: 139:9566026 CAPLUS
DOCUMENT NUMBER: 139:9566026 CAPLUS
DOCUMENT NUMBER: 139:9566026 CAPLUS John C: Loverine Perst.

131:199619
Preparation of indole derivatives as phospholipase
enzyme inhibitors
Seehra, Jashir S.; McKew, John C.; Lovering, Frank;
Bemis, Jean E.; Xiang, Yibin; Chen, Lihren; Knopf,
John L. INVENTOR (5):

John L.
Genetics Institute, Inc., USA
PCT Int. Appl., 182 pp.
CODEN: PIXXD2 PATENT ASSIGNEE(S):

DOCUMENT TYPE: LANGUAGE: English

L10 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: (Continued)

	PAT	ENT	ΝО.					DATE			APP	LICA	TIC	N I	١٥.		D.	ATE		
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241497-74-5P 241497-74-5P
RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation) of indole deriva. as phospholipase enzyme inhibitors for treatment of inflammatory conditions)

ANSWER 20 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 03 Sep 1994

AB Title compds. I (R1 = MeCHMe, MeCHF, HOCH2; R2 = H, C1-4 alkyl; Z = HO2C, HO3S, tetrazol-5-yl, C1-4alkyl-SO2HHCO; A = (substituted)Ph or thienyl) a pharmaceutically acceptable salt or in vivo hydrolyzable ester thereof, are prepared 2-Thiophenecarboxylic acid was nitated to give the 4-nitro derivative, reduced ti the 4-amino derivative converted to the (2S, 48)-1-(4-nitrobenzylcarbonyl)-2-(2-carboxy4-thienylcarbammyl)pyrrolidin-4-ylthloacetate which in in 4 steps was converted to SR, 6S, 8R, 2S, 4'S]-1 (R1 = MeCHMH, R2 = H, A = 4-thienyl, Z = 2-HO2C) which had a min. inhibitory concentration of 0.5 mg/mL against Enterobacter cloacae 108 vs 32 mg/L of ceftriaxone. Pharmaceutical formulations comprising I are given.

ACCESSION NUMBER: 1994:508368 CAPLUS
DOCUMENT NUMBER: 1994:508368 CAPLUS
TITLE: Preparation of antibiotic pyrrolidinylthiopenem derivatives

INVENTOR(S): Siret, Patrice Jean

Zeneca Ltd., UK; Zeneca Pharma S.A.

SOURCE: EXXDW

POCUMENT TYPE: Patent

LANGUAGE: ENXDW

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 592167	Al	19940413	EP 1993-307843	19931001
EP 592167	Bl	19991222		
R: AT, BE, CH,	DE, DK,	ES, FR, GB,	GR, IE, IT, LI, LU,	MC, NL, PT, SE
CA 2106330	AA	19940408	CA 1993-2106330	19930916
AT 187968	E	20000115	AT 1993-307843	19931001
ES 2140445	тэ	20000301	ES 1993-307843	19931001
JP 06211871	A2	19940802	JP 1993-250437	19931006
US 5538962	A	19960723	US 1993-132256	19931006
PRIORITY APPLN. INFO.:			EP 1992-402733	19921007
OTHER SOURCE(S):	MARPAT	121:108368		
IT 155481-27-9P 155481-	28-OP 15	6631-41-3P		

156631-42-4P

156631-42-4P
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, in preparation of antibiotics)
155481-27-9 CAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[{(5-carboxy-3-thienyl)amino]carbonyl]-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9CI)
(CA INDEX NAME) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 241497-74-5 CAPLUS
CN 3-Thiophenecarboxylic acid, 4-[[[5-[(cyclopentylcarbonyl)amino]-1(diphenylmethyl)-1H-indol-3-yl]carbonyl)amino]- (9CI) (CA INDEX NAME)

(Continued) L10 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN

155481-28-0 CAPLUS
1-Pyrrolidinecarboxylic acid, 2-[[(5-carboxy-3-thienyl)amino]carbonyl]-4-mercapto-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

 $\label{eq:continuous} $$156631-41-3$$ CAPLUS $$4-Thia-1-azabicyclo(3.2.0)$$ hept-2-ene-2-carboxylic acid, $$6-[1-[[(1,-dimethylethyl)dimethylsilyl]oxy]ethyl]-3-[[1-[((4-nitrophenyl)methoxy]carbonyl]-5-[[[5-[(2-propenyloxy)carbonyl]-3-thienyl]naino[carbonyl]-3-pyrrolidinyl]thio]-7-oxo, 2-propenyl ester, $$[5R-[3(3S^*,5S^*),5\omega,6\omega(R^*)]]-$$(CA INDEX NAME)$$$

Absolute stereochemistry.

156631-42-4 CAPLUS

L10 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 4-Thia-1-arabicyclo[3.2.0]hept-2-ene-2-carboxylic acid,
6-(1-hydroxyethyl)-3-[1[-[(4-nitrophenyl)methoxy]carbonyl]-5-[[[5-[(2-propenyloxy)carbonyl]-3-thienyl]mino[carbonyl]-3-pyrrolidinyl]thio]-7-oxo, 2-propenyl ester, [5R-[3(38*,58*),5a,6a(R*)]]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

	AT 185140	E	19991015	AT	1993-906740		19930324
	ES 2136124	T3	19991116	ES	1993-906740		19930324
	CA 2108356	C	20040120	CA	1993-2108356		19930324
	CN 1077957	A	19931103	CN	1993-102800		19930326
	CN 1036713	В	19971217				
	NO 9304264	A	19931125	NO	1993-4264		19931125
	FI 104075	B1	19991115	FI	1993-5245		19931125
	US 5519015	A	19960521	US	1993-142459		19931126
PRIO	RITY APPLN. INFO.:			EP	1992-400836	А	19920326
				EΡ	1992-402763	А	19921009
				WO	1993-GB603	А	19930324
OTHE	R SOURCE(S):	MARPAT	121:9029				
IT	155481-26-8P 155481-2	27-9P 1	55481-28-0P				
	155481-30-4P 155481-3	31-5P 1	55481-32-6P				
	RL: RCT (Reactant);	SPN (S	vnthetic pre	par	ation); PREP (Pr	epar	ation); RACT
	(Reactant or reagent		•	•		•	
	(preparation and	reacti	on of, in pr	epa	ration of		
carb	oxythienylcarbamovlpy						
	ylthiocarbapenemo						
RN	155481-26-8 CAPLUS						
CN	1-Azabicyclo[3.2.0]h	ept-2-	ene-2-carbox	vli	c acid. 3-[15-[[(5-c	arboxv-3-
	thienyl) amino] carbon						
	pyrrolidinyl[thio]-6						-
	2-{(4-nitrophenyl)me					(
	R*)]]-, compd. with						1:1) (9CI)
	(CA INDEX NAME)				.,		
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L10 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CRN 155481-25-7 CMF C35 H33 N5 O13 S2

CM 1

CM 2 CRN 7087-68-5 CMF C8 H19 N L10 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 09 Jul 1994

AB Title compds. I {R = {un}substituted carboxythienyl; Rl = CHMeOH, CHMeF, CHZOH; R2, R3 = H, alkyl} were prepared Thus, the carbapenem II was obtained from the diphenylphosphoryloxycarbapenem and the thiol, prepared from 2-thiophenecarboxylic acid and the protected mercaptopytrolidinecarboxylic acid in 4 steps. II had min. inhibitory concns. against Staphylococcus aureus Oxford 0.125 and Escherichia coli DCO 0.008 µg/mL.

ACCESSION NUMBER: 1994:409029 CAPLUS
DCCUMENT NUMBER: 121:9029

TITLE: Carbapenem derivatives as antibiotics and intermediates thereof

1994:409029 CAPLUS
121:9029
Carbapenem derivatives as antibiotics and intermediates thereof
Jung, Frederic Henri
Zeneca Ltd., UK: Zeneca Pharma S. A.
PCT Int. Appl., 44 pp.
CODEN: PIXXD2
Patent

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA'	TENT	NO.			KIN	D	DATE			APP	LIC	AT:	ION I	10.		D.	ATE		
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WO	9319	070			A1		1993	0930		WO	199	3-0	GB60:	3		1	9930	324	
	W:	AT,	AU,	BB,	BG,	BR,	CA,	CH,	CZ,	DΕ	, D	ĸ,	ES,	FI,	GB,	HU,	JP,	KP,	
		KZ,	LK,	LU,	MG,	NL,	NO,	PL,	RO										
	RW:	AT,	BE,	CH,	DE.	DK,	ES.	FR,	GB,	GR	, I	E,	IT,	LU,	MC,	NL,	PT,	SE,	
		BF.	BJ,	CF,	CG,	CI.	CM,	GA,	GN,	ML									
ZA	9301	611			A		1993	0927		ZA	199	3-	1611			1	9930	305	
IL	1051	35			A1		2000	0131		IL	199	3-	1051	35		1	9930	323	
ΑU	9337	636			A1		1993	1021		ΑU	199	3-3	3763	6		1	9930	324	
AU	6629	72			B2		1995	0921											
EP	5866	63			A1		1994	0316		ĔΡ	199	3-	9067	40		1	9930	324	
EP	5866	63			B1		1999	0929											
	R:	AT.	BE.	CH,	DE,	DK,	ES,	FR,	GB,	GR	, I	Ε,	IT,	LI,	LU,	MC,	NL,	PT,	SE
ΗU	6571	3 .			A2		1994	0728		HU	199	3-	3304			1	9930	324	
JP	0650	8372			T2		1994	0922		JΡ	199	3-	5163	98		2	9930	324	
10	2212	266			82		2002	0812											

L10 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

155481-27-9 CAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[{5-carboxy-3-thienyl}amino]carbonyl]-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155481-28-0 CAPLUS
1-Pyrrolidinecarboxylic acid, 2-[[(5-carboxy-3-thienyl)amino]carbonyl]-4-mercapto-, 1-[(4-mitrophenyl)methyl] ester, (28-cis)- (9CI) (CA INDEX

Absolute stereochemistry.

155481-30-4 CAPLUS 155481-30-4 CAPLUS

1-Azabicyclo[3].2.0]hept-2-ene-2-carboxylic acid, 3-[[5-[[(2-carboxy-3-thienyl)amino]carbonyl]-1-[[(4-nitrophenyl)methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-[1-hydroxyethyl]-4-methyl-7-oxo-, 2-[2-propenyl) ester, [4R-[3](38).55); (40,5],6](R*)]]-, compd. with N-ethyl-N-[1-methylethyl]-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CRN 155481-29-1 CMF C31 H32 N4 O11 S2

Absolute stereochemistry.

CM 1

CM 2 CRN 7087-68-5 CMF C8 H19 N

Ęt i-Pr-N-Pr-i

155481-31-5 CAPLUS 137401313 Artists
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-{{(2-carboxy-3-thienyl)amino[carboxyl]-, 1-{(4-nitrophenyl)methyl) ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155481-32-6 CAPLUS 1-Pyrrolidinecarboxylic acid, 4-mercapto-2-[(3-thienylamino)carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 29 Nov 1991

$$CH_2O_2C-N$$

$$COR$$

$$I$$

$$Q^1 = -NH$$

$$S$$

Title compds. I [R = 5- or 6-membered (monohydroxylated) (O- or S-containing) saturated cyclic amino, Q, Q1], useful for treatment of amnesia and dementia, are prepared Treatment of carbobenzoxy-L-pyroglutamic acid with thiazolidine, 1-hydroxybenztriazole.H2O, and DCC in MeCN at room temperature

thiazolidine, 1-hydroxybenztriazole.H2O, and DCC in MeCN at room temperation

14 h gave N-(1-benzyloxycarbonyl-5-oxo-L-prolyl)thiazolidine, which inhibited prolyl endopeptidase with LC50 of 0.32 µM.

ACCESSION NUMBER: 1991:632874 CAPLUS

DOCUMENT NUMBER: 115:232874

Preparation of pyroglutamic acid amides as prolyl endopeptidase inhibitors

INVENTOR(S): Purukawa, Ataushi: Yoshimoto, Tadashi: Tsuru, Onori; Ajiaawa, Yukiyoshi: Kinoshita, Yukihiko

PATENT ASSIGNEE(S): Kissei Pharmaceutical Co., Ltd., Japan

Jon. Kokai Tokkyo Koho, 7 pp.

CODDINENT TYPE: DOCUMENT TYPE: Patent

LANGUAGE: Japanse

PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE PATENT NO. KIND DATE APPLICATION NO. DATE

JP 03056461 A2 19910312 JP 1989-190747 19890724

JP 07103101 B4 19951108 JP 1989-190747 19890724

PRIORITY APPLN. INFO.: JP 1989-190747 19890724

OTHER SOURCE(S): MARPAT 115:232874

IT 137042-90-1P (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of, as prolyl endopeptidase inhibitor)

RN 137042-90-1 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-oxo-5-{{(tetrahydro-2-oxo-3-thienyl)amino[carbonyl]-, phenylmethyl ester, (S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L10 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

=> s 16

L11 2 L6

=> d ed abs ibib hitstr 1-2

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 27 Jul 2001

AB The title compds. [I; X = O, S: Rl = alkyl, cycloalkyl, halo; R2 = H, alkyl, alkoxy, etc.; R3 = alkyl; A = (un)substituted ortho-substituted (hetero)aryl, bicyclo(hetero)aryl) which have plant-protective properties and are suitable for protecting plants against infestations by phytopathogenic microorganisms, were prepared Thus, methylation of Me 4-methylpyrcole-3-carboxylate followed by hydrolysis of the resulting ester, and reaction of 1,4-dimethylpyrrole-3-carboxylic acid with 2-(4'-fluorob)henyl)aniline afforded I [X = O; Rl, R3 = Me; R2 = H; A = 4'-fluorob)henyl-2-yl] which showed strong efficacy against Puccinia recondita on wheat (< 20% infestation).

ACCESSION NUMBER: 2001:545661 CAPLUS
DOCUMENT NUMBER: 135:137397
Preparation of pyrrolecarboxamides and pyrrolethioamides as fungicides
INVENTOR(S): Walter, Harald's Chemieder, Hermann
Syngenta Participations A.-G., Switz.

PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Esplish

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION

PA'	FENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE	
						-									-		
WO	2001	0532	59		A1		2001	0726	,	WO 2	001-	EP59	2		2	0010	119
	W:	AE,	AG.	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR.	BY.	BZ.	CA,	CH,	CN,
								DZ,									
								KE,									
		LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ.	NO.	NZ.	PL.	PT.	RO.	RU,
								TJ,									
		YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM				
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		BJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
	2397																
BR	2001	0077	38		А		2002	1022		BR 2	001-	7738			2	0010	119
EΡ	1252	140			Al		2002	1030		EP 2	001-	9074	68		2	0010	119
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	TI,	LI,	LU,	NL,	SE,	MC,	PT,
								MK,									
JP	2003	5202	69		T2		2003	0702		JP 2	001-	5532	63		2	0010	119
	7726															0010	119
ZA	2002	0056	41		А		2003	1103		ZA 2	002-	5641			2	0020	715

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS On STN
US 2004049035 A1 20040311 US 2002-181702 US 2004049035 US 6806286 A1 B2 20040311 20041019 20021008 US 2004106521 US 2003-680346 20040603 20031007 GB 2000-1447 WO 2001-EP592 US 2002-181702 PRIORITY APPLN. INFO .: 20000121 20010119 A3 20021008

OTHER SOURCE(S): MARPAT 135:137397 IT 351416-74-5P 351416-75-6P 351416-76-7P

351416-74-59 351416-75-6P 351416-76-PP
RL: AGR (Agricultural use): BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation): USES (Uses) (preparation of pyrrolecarboxamides and pyrrolethioamides as fungicides) 351416-74-5 CAPLUS
H-Pyrrole-3-carboxamide, N-[2-{4-chlorophenyl}-3-thienyl}-1,4-dimethyl-(9CI) (CA INDEX NAME)

351416-75-6 CAPLUS
1H-Pyrrole-3-carboxamide, N-[2-(4-chlorophenyl)-3-thienyl]-1-methyl-4(pentafluoroethyl)- (9CI) (CA INDEX NAME)

351416-76-7 CAPLUS

1H-Pyrrole-3-carboxamide, N-[2-(4-fluorophenyl)-3-thienyl]-1-methyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 25 Feb 2000

Title compds. I (R1 = H, halo, alkyl, haloalkyl; R2 = alkyl, haloalkyl, alkoxyalkyl, cyano, alkylsulfonyl, arylsulfonyl, etc.; A = substituted Ph, substituted 3-thienyl, substituted 4-indanyl) were prepared as plant protectants. Thus, 1.9 gl-methyl-4-(trifluoromethyl)pyrrole-3-carboxylic acid, obtained from Et 4,4.4-trifluorocrotonate, tosylmethyl isocyanide, and MeI, and 0.9 mL oxalyl chloride in 20 mL CH2C12 was stirred at room temperature in the presence of a catalytic amount of DMF, the solvent was pocated

evaporated
under reduced pressure to give a crystalline solid, and the solid was added to
a solution of 1.7 g of 2-biphenylamine and 4.2 mL Bt3N in 20 mL CH2Cl2 at
0°, and the reaction mixture was stirred for 2 h at room temperature to
give I (Rl = H, R2 = Me, A = 2-biphenylyl). Application of this compound on
apples, grapes, and tomatoes resulted in <10% infestation by Botrytis
clinera.
ACCESSION NUMBER: 2000:133660 CAPLUS

2000:133660 CAPLUS
132:166122
(Trifluoromethyl)pyrrolecarboxamides
Eberle, Martin; Walter, Harald
Novartis A.-G., Switz.; Novartis-Erfindungen
Verwaltungsgesellschaft m.b.H.
PCT Int. Appl., 35 pp.
CODEN: PIXXD2 DOCUMENT NUMBER: TITLE: INVENTOR(S): PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO. WO 2000009482 TW 576831 AU 9955138 AU 756140 EP 1105375 A1 20010508 BR 1999-12962 19990810
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
TR 200100478 T2 20010621 TR 2001-200100476

Lll	ANSWER 2 OF 2 CF	APLUS CO	PYRIGHT 2005	ACS	on STN (C	Continu	ed)
	JP 2002522526	T2	20020723	JP	2000-564936		19990810
	US 2002019541	Al	20020214	US	2001-780897		20010209
	US 6365620	B2	20020402				
PRIC	RITY APPLN. INFO. :			GB	1998-17548	А	19980812
				WO	1999-EP5837	W	19990810
OTHE	R SOURCE(S):	MAR PA	T 132:166122				
IΤ	258510-88-2P 2585	10-89-3P	258510-91-7P				
IT					except advers	se); BSI	U (Biologica
IT	RL: BAC (Biologic	al activ	ity or effec	tor,			
IT	RL: BAC (Biologic study, unclassifi	al activ	ity or effect (Synthetic	tor,			
IT	RL: BAC (Biologic study, unclassifi study); PREP (Pre	al actived): SPN	ity or effect (Synthetic	tor,	aration): BIO	L (Biol	ogical
TT RN	RL: BAC (Biologic study, unclassifi	al actived): SPN paration hyl)pyrr	ity or effect (Synthetic	tor,	aration): BIO	L (Biol	ogical
	RL: BAC (Biologic study, unclassifi study); PREP (Pre ((trifluoromet	ed): SPN paration hyl)pyrr	ity or effec (Synthetic) olecarboxami	tor, prepa	aration): BIOI	L (Biole	ogical)

RN 258510-89-3 CAPLUS
CN 1H-Pyrcole-3-carboxamide, N-{2-(4-chlorophenyl)-3-thienyl}-1-methyl-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 258510-91-7 CAPLUS
CN 1H-Pyrrole-3-carboxamide, N-(2-[1,1'-biphenyl]-4-yl-3-thienyl)-1-methyl-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

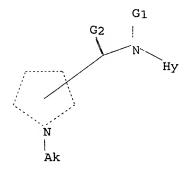
REFERENCE COUNT:

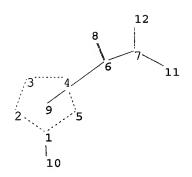
THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Page 4230/08/2005

=> log y
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE
-18.25

STN INTERNATIONAL LOGOFF AT 12:06:27 ON 30 AUG 2005





chain nodes:
6 7 8 10 11 12
ring nodes:
1 2 3 4 5
chain bonds:
1-10 6-7 6-8 7-11 7-12
ring bonds:
1-2 1-5 2-3 3-4 4-5
exact/norm bonds:

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-12

G1:H,CH3

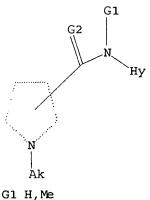
G2:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:CLASS
Generic attributes:
11:

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



GI H, ME

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s 11 SAMPLE SEARCH INITIATED 13:44:46 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 136055 TO ITERATE

1.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

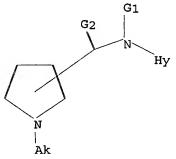
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

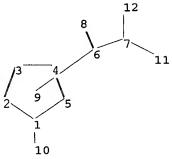
PROJECTED ITERATIONS: 2699331 TO 2742869 PROJECTED ANSWERS: 8214 TO 10832

L2 7 SEA SSS SAM L1

=>

Uploading C:\Program Files\Stnexp\Queries\10680346exp2.str





7 ANSWERS

chain nodes:
6 7 8 10 11 12
ring nodes:
1 2 3 4 5
chain bonds:
1-10 6-7 6-8 7-11 7-12
ring bonds:
1-2 1-5 2-3 3-4 4-5
exact/norm bonds:

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-12

G1:H,CH3

G2:0,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS

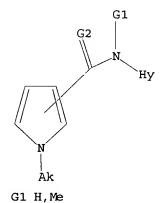
11:Atom 12:CLASS Generic attributes :

11:

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

L3 STRUCTURE UPLOADED

=> d 13 L3 HAS NO ANSWERS L3 STR



Structure attributes must be viewed using STN Express query preparation.

7 ANSWERS

=> s 13

G2 0,S

SAMPLE SEARCH INITIATED 13:46:21 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 136055 TO ITERATE

1.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

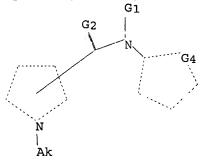
BATCH **INCOMPLETE**

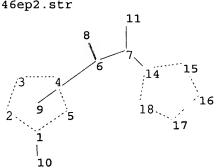
PROJECTED ITERATIONS: 2699331 TO 2742869 PROJECTED ANSWERS: 8214 TO 10832

L4 7 SEA SSS SAM L3

=>

Uploading C:\Program Files\Stnexp\Queries\346ep2.str





chain nodes : 6 7 8 10 11

ring nodes :

1 2 3 4 5 14 15 16 17 18

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-15 14-18 15-16 16-17 17-18

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-15 14-18 15-16 16-17 17-18

G1:H, CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

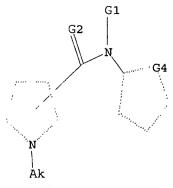
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G1 H, Me

G2 0,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 13:52:22 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1828 TO ITERATE

100.0% PROCESSED 1828 ITERATIONS

11 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 33996 TO 39124

PROJECTED ANSWERS: 22 TO 418

L6 11 SEA SSS SAM L5

=> s 15 full

FULL SEARCH INITIATED 13:52:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 37137 TO ITERATE

100.0% PROCESSED 37137 ITERATIONS 294 ANSWERS

SEARCH TIME: 00.00.01

L7 294 SEA SSS FUL L5

=> fil hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 166.92 167.13

FILE 'HCAPLUS' ENTERED AT 13:52:44 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17 L8 41 L7

=> d ed abs ibib hitstr 1-41

ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 13 May 2005

Title compds. I [wherein R1 = (un)substituted (C3-7 cycloalkyl)methyl, hetero/arylr R2 = H, NO2, CN, CO2H and derivs., NH2 and derivs., etc.; R3 = (un)substituted hetero/aryl; and their pharmaceutically acceptable salts] were prepared as p38 MAP kinase inhibitors for treating and/or preventing immune or infilammatory disorders. For example, II was prepared by reacting Et 3-brome-6-oxo-7-phenyl-6,7-dihydrothieno(2,3-b)pyridine-2-carboxylate (preparation given) with 3-methylbenzaldehyde and oxidation with

MnO2.

I are potent inhibitors of p38 MAP kinase (IC50 around 2 µM and below),
especially p38c kinase.

ACCESSION NUMBER:
DOCUMENT TYPE:
DOCUMENT TYPE:
PATENT ASSIGNEE(S):
SOURCE:
POTENT ASSIGNEE(S):
DOCUMENT TYPE:
PATENT ASSIGNEE(S):
DOCUMENT TYPE:
DOCUMENT TY

FAMILY ACC. NUM. COUNT:

(Continued) ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

851753-37-2P, N-(3-Benzoyl-6-oxo-7-phenyl-6,7-dihydrothieno(2,3-b)pyridin-2-yl)-1-methyl-2-pyrrolidinecarboxamide 851753-40-7P, N-(3-Benzoyl-6-oxo-7-phenyl-6,7-dihydrothieno[2,3-b)pyridin-2-yl)-1-methyl-D-prolinamide

RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(p38e kinase inhibitor: preparation of thienopyridinones as p38 MAP kinase inhibitors useful in the treatment of and/or prevention of immune or inflammatory disorders)
851753-37-2 KCAPLUS
2-Pyrrolidinecarboxamide, N-(3-benzoyl-6,7-dihydro-6-oxo-7-phenylthieno[2,3-b]pyridin-2-yl)-1-methyl-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

851753-40-7 RCAPLUS
2-Pyrrolidinecarboxamide, N-(3-benzoyl-6,7-dihydro-6-oxo-7-phenylthieno(2,3-bl)pyridin-2-yl)-1-methyl-, (2R)- [9CI) (CA INDEX NAME)

Absolute stereochemistry.

L0 ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN PATENT INFORMATION: (Continued)

PAT	ENT	NO.			KIN	D	DATE			APPL	I CAT	ION :	NO.		D	ATE	
						-									-		
WO	2005	0425	40		A1		2005	0512	1	WO 2	004-	GB 4 4	90		2	0041	022
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		CN,	co,	CR.	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
		LK.	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK.	MN.	MW,	MX.	MZ,	NA,	NI,
		NO.	NZ,	OM,	PG,	PH,	PL,	PT.	RO.	RU,	sc,	SD.	SE,	SG,	SK.	SL,	SY,
		TJ.	TM.	TN.	TR,	TT.	TZ.	UA.	UG,	US,	UZ.	VC.	VN,	YU.	ZA,	ZM.	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ.	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE.	BG,	CH,	CY.	CZ,	DE,	DK,
		EE.	ES,	FI,	FR,	GB,	GR,	Hυ,	IE,	IT,	LU,	MC.	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
			TD,														

PRIORITY APPLN. INFO.:

20031024 20031219 20040210 20040729

OTHER SOURCE(S): MARPAT 142:463710

THER SOURCE(S): MARPAT 142:463710

S51749-00-JP, tert-Butyl (2S)-2-{[(3-benzoyl-6-oxo-7-phenyl-6, 7-dihydrothieno[2,3-b]pyridin-2-yl)amino]carbonyl]pyrrolidine-1-carboxylate

S51749-02-SP, tert-Butyl (2R)-2-{[(3-benzoyl-6-oxo-7-phenyl-6, 7-dihydrothieno[2,3-b]pyridin-2-yl)amino]carbonyl]pyrrolidine-1-carboxylate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(intermediate; preparation of thienopyridinones as p38 MAP kinase inhibitors useful in the treatment of and/or prevention of immune or inflammatory disorders)

RN 851749-00-3 HCAPLUS

N1 -Pyrrolidinecarboxylic acid, 2-{[(3-benzoyl-6,7-dihydro-6-oxo-7-phenylthieno[2,3-b]pyridin-2-yl]amino]carbonyl]-, 1,1-dimethylethyl ester,

(2S)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

851749-02-5 HCAPLUS
1-Pyrrolidinecarboxylic acid, 2-{{{3-benzoyl-6,7-dihydro-6-oxo-7-phenylthieno(2,3-b]pyridin-2-yl}amino]carbonyl}-, 1,1-dimethylethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 06 Aug 2004

Condensed pyridines and pyrimidines (quinolines, quinazolines and thienopyrimidines) of formula I [X is N or CH: Y is -NR- or -NHCH2-; R is alkyl: A is a fused 5-7 membered carbocyclic or N/O/S-heterocyclic ring with one or more RI groups; RI is H, halo, NOZ, alkyl, OR, CONRARS, O(CH2)nNRARS, OR NRARS; R2 is certain N-containing heterocyclic rings; R3 is pyridin-2-yl, CI-6alkyl-pyridin-2-yl, -pyrrol-2-yl or -thiazol-2-yl; R4 is H or alkyl; R5 is alkyl: NRARS can be 3-7 membered (un)saturated N/O/S-heterocycle] and their pharmaceutically acceptable salts, solvates or derivs. were synthesized. Thus, 2-aminobenzamide was coupled with 6-methyl-2-pyridinecarboxylic acid in the presence of EDCI/HOBT followed by cyclocondensation mediated by NaOH to give quinazolinone II. Chlorination of III with POCI3 and subsequent substitution of the resulting chloride with 4-aminopyridine afforded quinazoline III. These compds. are inhibitors of the transforming growth factor TGF-P, especially of activin-like kinase ALK-5 receptor, and are used in the treatment and prevention of Various disease states mediated by ALK-5 kinase mechanisms such as kidney fibrosis. All the final products showed ALK5 receptor modulator activity with ICSO of 0.001-10 µM (82 nM for III). The role of ALK5 inhibitors for the treatment of photoaging was also demonstrated exptl.

SION NUMBER: 2004:633933 HCAPUS

expt1. ACCESSION NUMBER: MENT NUMBER:

2004:633933 HCAPLUS 141:174181

Preparation of quinolines, quinazolines and thienopyrimidines as ALK-5 receptor ligands for the treatment of kidney fibrosis Dodic, Nerina; Gellibert, Francoise Jeanne; Hunter,

INVENTOR (S):

EN ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

EN Entered STN: 19 Jul 2004

AB Hairpin polyamides are synthetic oligomers, which fold and bind to specific DNA sequences in a programmable manner. Internal side-by-side pairings of the aromatic amino acid residues 1-methyl-1H-pyrrole (Fy), 1-methyl-1H-imidazole [Imi, and 3-hydroxy-1-methyl-1H-pyrrole (Fy), 1-methyl-1H-imidazole [Imi, and 3-hydroxy-1-methyl-1H-pyrrole (Hp) confer the ability to distinguish between all 4 Watson-Crick base pairs in the minor groove of B-form DNA. In a broad search to expand the heterocycle repertoire, we found that when 3-methylthiophene (Th), which presents a S-atom to the minor groove, is paired with Fy, it exhibits a modest 3-fold specificity for T-A > A-T, presumably by shape-selective recognition. In this study, we explore the scope and limitations of this lead by incorporating multiple Tn residues within a single hairpin polyamide. Hairpin polyamides containing >1 Tn/Py pair exhibit lowered affinities and specificities for their match sites. It appears that little deviation is permissible from the parent 5-membered ring 1-methyl-1H-pyrole-2-carboxamide scaffold for DNA recognition.

ACCLESSION NUMBER: 2004:573249 HCAPLUS

DNA minor-groove recognition by 3-

TITLE:

AUTHOR (S):

141:407378

DNA minor-groove recognition by 3-methylthiophene/pyrrole pair
Doss, Raymond M.: Marques, Michael A.: Foister, Shane;
Dervan, Peter B.
Division of Chemistry and Chemical Engineering,
California Institute of Technology, Pasadena, CA,
91125, USA
Chemistry & Biodiversity (2004), 1(6), 886-899
CODEN: CBMIAN; ISSN: 1612-1872
Verlag Helvetica Chimica Acta AG
Journal
English CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

791626-78-32

PSI 522-78-3P
RL: ARG (Analytical reagent use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process); USES (USES) (USA) (DNA minor-groove recognition by 3-methylthiophene/pyrrole pair) 791626-78-3 HCAPLUS (Cidmethylamino)propyl) amino]-3-oxopropyl) amino|carbonyl]-1-methyl-1H-pyrrol-3-yl]amino|carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-4-{[4-[[1-methyl-4-[[3-methyl-5-[[1-methyl-4-[4-[1-methyl-3-

L8 ANSWER 2 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN
ROBERT Neil, III
PATENT ASSIGNEE(S): SNIKELINE SECCION COPPORATION, USA
PCT Int. Appl., 50 pp.
CODEN: PIXXD2 (Continued)

DOCUMENT TYPE: Patent

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ENT I	ю.			KIN	D	DATE			APPL	ICAT	ION	NO.		DI	ATE	
						-											
WO :	2004	0653	92		Al		2004	0805	1	WO 2	004-	EP65	0		21	0040	126
WO :	2004	0653	92		C1		2004	1007									
	W:	ΑE,	ΑE,	AG,	AL,	AL,	AM,	AM,	AM,	AT,	AT,	ΑU,	ΑZ,	AZ,	BA,	ВB,	BG,
		BG,	BR,	BR,	BW,	BY,	BY,	BZ,	ΒZ,	CA,	CH,	CN,	CN,	co,	co,	CR,	CR,
		CU,	CU,	CZ,	CZ,	DE,	DE,	DK,	DK,	DM,	DZ,	EC,	EC,	EE,	EE,	EG.	ĒS,
		ES,	FI,	FI,	GB,	GD,	GE,	GE,	GH,	GM,	HR,	HR,	HU,	Hυ,	ID,	IL,	IN,
		IS,	J₽,	JP,	ΚE,	ΚE,	KG,	KG,	KP,	KP,	KP,	KR,	KR,	ΚZ,	ΚZ,	ΚZ,	LC,
		LK,	LR,	LS,	LS,	LT,	LU,	LV,	MA,	MD,	MD,	MG,	MK,	MN,	MW,	MX,	MX,
		MZ,	MZ,	NA,	NI												
PRIORITY	APP	LN.	INFO	. :						GB 2	003-	1719			A 20	0030	124

OTHER SOURCE(S): MARPAT 141:174181

T 733805-35-47

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate: preparation of quinolines, quinazolines and thienopyrimidines as ALK-5 receptor ligands for the treatment of, e.g., kidney fibrosis)

RN 733806-35-4 RCAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[3-(aminocarbonyl)-4-methyl-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

GB 2003-8706

A 20030415 A 20030702

REFERENCE COUNT:

2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

PAGE 2-A

791626-83-0P 791626-84-1P 791626-85-2P
RL: PRP (Properties): PUR (Purification or recovery): RCT (Reactant): SPN
(Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(DNA minor-groove recognition by 3-methylthiophene/pyrrole pair)
791626-83-0 HCAPLUS

791626-83-0 HCAPLUS
2-Thiophenecarboxylic acid, 3-methyl-5-[[(1-methyl-4-nitro-1H-pyrrol-2-

ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) y1)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

2-Thiophenecarboxylic acid, 5-[[[4-[([1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-3-methyl-, methyl ester (9CI) (CA INDEX NAME)

791626-85-2 HCAPLUS 2-Thiophenecarboxylic acid, 5-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-3-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN DOCUMENT TYPE: Patent English FAMILY ACC. NUM. COUNT: 1 (Continued)

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2004039799 A1 20040513 WO 2003-EP11805 20031024

W: AL, AG, AL, AM, AT, AL, AZ, BB, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LS, LT, LU, LV, NA, MD, MG, MK, MN, MK, MX, NX, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, ZZ, UA, UG, US, UZ, VC, VV, VU, ZA, ZM, ZW, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, SF, BJ, CP, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG
CA 2501739 AA 20040513 CA 2003-2501739 20031024

EP 1556377 A1 20050727 EP 2003-776869 20031024

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRIORITY APPLN. INFO:

MARPAT 140:406731 PATENT NO. KIND DATE APPLICATION NO. DATE

PRIORITY APPIN. INFO.:

OTHER SOURCE(S):

MARPAT 140:406731

IT 688324-04-1P 6889324-05-2P 688324-06-3P
688324-10-1P 6889324-05-89 688324-06-6P
688324-10-9P 6889324-11-0P 688924-12-1P
688324-13-2P 6889324-11-0P 688924-12-1P
688324-13-2P 6889324-17-6P 688924-12-1P
688324-19-8P 689324-17-6P 688924-12-1P
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688324-23-9P 689324-23-4P 688924-24-5P
688324-23-PP 689324-25-6P 688924-27-8P
688324-31-4P 689324-35-6P 688924-30-3P
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689324-30-3P 689324-36-PP 688924-45-PP
689324-43-PP 689324-45-PP 688924-45-PP
689324-50-7P 689324-56-PP 688924-55-PP
689324-56-3P 689324-55-PP 688924-55-PP
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689324-66-PP 689324-56-PP 688924-61-PP
689324-66-PP 689324-56-PP 688924-76-PP
689324-74-5P 689324-78-PP 688924-77-PP
689324-74-5P 689324-78-PP 688924-77-PP
689324-74-5P 689324-78-PP 6889324-78-PP
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689324-74-5P 689324-78-PP 689324-78-PP
689324-74-5P 689324-78-PP
689324-78-P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES

(uses)
(fungicide: preparation of N-(cyclopropylthienyl)carboxamides as fungicides)
688324-04-1 RCAPUS
HH-Pyrrole-3-carboxamide, N-[3-(2-ethylcyclopropyl)-2-thienyl]-1-methyl-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 13 May 2004

A fungicidally active compound I, II, or III [wherein Het = (un) substituted 5- or 6-membered heterocyclic ring containing one to three O, N, and/or S atoms, provided that the ring is not 1,2,3-triazole: Rl and R2 independently H, halo, or Mer. R3 = (un) substituted (cyclo)alkyl, alkenyl, alkynyl. Ph, heterocyclyl: R7 and R8 = independently H, halo, or (halo)alkyl) were prepared for use as active ingredients in agricultural or hotticultural compns. for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. For example, 3-difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid was amidated with [2-(bicyclopropyl-2-yl) thiophen-3-yl] amine in the presence of TEA and N,N-bis(2-oxooxazolidinyl)phosphinic acid chloride in CH2C12 to give trans-IV [97s purity]. The latter showed excellent activity against Puccinia recondita on wheat (0-5% infestation) and showed good activity against Podosphaera leucotricha on apple, Venturia inaequalis on apple, Erysiphe graminis on barley, Pyrenophora teres on barley, Alternaria solani on tomato, and Uncinula necator on grape (<20% infestation for each).

each).
ACCESSION NUMBER:
DOCUMENT NUMBER:
TITLE: 2004:390242 HCAPLUS 140:406731

Preparation of N-(cyclopropylthienyl)carboxamides as fungicides

Lungucides
Ehrenfreund, Josef: Tobler, Hans: Walter, Harald
Syngenta Participations Ag, Switz.
PCT Int. Appl., 43 pp.
CODEN: PIXXO2

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688324-05-2 HCAPLUS
1H-Pyrrole-3-carboxamide, N-[3-(2-ethylcyclopropyl)-2-thienyl]-1(methoxymethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-06-3 HCAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-(2-propylcyclopropyl)-2-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

688324-07-4 HCAPLUS 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-(2-propylcyclopropyl)-2-thienyl]- (9CI) (CA INDEX NAME)

688324-08-5 HCAPLUS
1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-[2-(1-methylethyl)cyclopropyl]-2-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-09-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-[2-(1-methylethyl)cyclopropyl]-2-thienyl]- (9CI) (CA INDEX NAME)

RN 688324-10-9 HCAPLUS
CN 1H-Pyrclol-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-(3-[2-(1-methylethyl)-cylopropyl]-2-thienyl]- (9C1) (CA IMDEX NAME)

RN 688324-11-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-[3-[2-(1-methylethyl)eyclopropyl]-2-thlenyl]- (9CI) (CA INDEX NAME)

RN 688324-12-1 HCAPLUS

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-16-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-butylcyclopropyl)-2-thienyl]-1-methyl-4(trifluoromethyl)- (SCI) (CA INDEX NAME)

RN 688324-17-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-butylcyclopropyl)-2-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-18-7 HCAPLUS CN 1H-Pyrrole-3-carboxamide, N-[3-(2-butylcyclopropyl)-2-thienyl]-2-fluoro-1.4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-19-8 HCAPLUS
CN 1H-Pyrcle-3-carboxamide, N-[3-(2-butylcyclopropyl)-2-thienyl]-2-chloro1,4-dimethyl- (9C1) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1-ethyl-4-methyl-N-[3-[2-{1-methylethyl}cyclopropyl]-2-thienyl]- (9CI) (CA INDEX NAME)

RN 688324-13-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-{3-{2-{1-methylethyl)cyclopropyl}-2-thienyl}- (9CI) (CA INDEX NAME)

RN 688324-14-3 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-ethyl-2-fluoro-4-methyl-N-[3-{2-(1-methylethyl)cyclopropyl}-2-thienyl}- (9CI) (CA INDEX NAME)

RN 688324-15-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-2-fluoro-1-methyl-N-[3[2-(1-methylethyl)cyclopropyl]-2-thienyl]- (SCI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-20-1 HCAPLUS
CN HH-Pyrrole-3-carboxamide, 1-methyl-N-(3-[2-(2-methylpropyl)cyclopropyl]-2thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-21-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-[2-(2-methylpropyl)cyclopropyl]-2-thienyl)- (9CI) (CA INDEX NAME)

RN 688324-22-3 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-{3-{2-(2-methylpropyl)cyclopropyl}-2-thienyl}- (9CI) (CA INDEX NAME)

RN 688324-23-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(methoxymethyl)-N-{3-[2-(2-methylpropyl)cyclopropyl]-2-thienyl]-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-24-5 HCAPLUS
(N H-Pyrrole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-(3-[2-(2-methylpropyl)cyclopropyl)-2-thienyl|- (9C1) (CA INDEX NAME)

RN 688324-25-6 HCAPLUS CN 1H-Pyrrol-3-carboxamide, 2-chloro-1,4-dimethyl-N-[3-[2-{2methylpropyl)-cyclopropyl]-2-chlenyl]- (9CI) (CA INDEX NAME

RN 688324-26-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-(1,1-dimethylethyl)cyclopropyl]-2-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-31-4 HCAPLUS CN H-Pyrrole-3-carboxamide, 1-methyl-N-[3-(2-pentylcyclopropyl)-2-thienyl]-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

RN 688324-32-5 HCAPLUS
CN IH-Pyrrole-3-carboxamide, 1-methyl-N-(3-[2-(3-methylbutyl)cyclopropyl]-2thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ &$$

RN 688324-33-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-{2-(3-methylbutyl)cyclopropyl]-2-thienyl]- (9CI) (CA INDEX NAME)

RN 688324-34-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-hexylcyclopropyl)-2-thienyl]-1-methyl-4(trifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 688324-27-8 HCAPLUS
CN 1H-Pytrole-3-carboxamide, 4-{difluoromethyl}-N-{3-{2-(1,1-dimethylethyl)cyclopropyl}-2-thienyl}-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-28-9 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-(1,1-dimethylethyl)cyclopropyl]-2thienyl]-2-fluoro-1,4-dimethyl- (9C1) (CA INDEX NAME)

RN 688324-29-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-[3-[2-(1,1-dimethylethyl)cyclopropyl]2-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-30-3 KCAPLUS
CN 1H-Pytrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-{3-[2-(1,1-dimethylethyl)cyclopropyl]-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-35-8 HCAPLUS CN H-Pyrrole-3-carboxamide, N-{3-{1,1'-bicyclopropy}}-2-yl-2-thienyl}-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-36-9 HCAPLUS
CN lH-Pyrrole-3-carboxamide, N-(3-[1,1'-bicyclopropy])-2-yl-2-thienyl)-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-37-0 HCAPLUS CN 1H-Pytrole-3-carboxamide, N-(3-[1,1'-bicyclopropyl]-2-yl-2-thienyl)-2fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-38-1 HCAPLUS CN 1H-Pytrole-3-carboxamide, N-(3-[1,1'-bicyclopropyl]-2-yl-2-thienyl)-2chloro-1,4-dimethyl- (9CI) (CA INDEX NAME)

LB ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

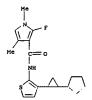
RN 688324-39-2 HCAPLUS CN 1H-Pytrole-3-carboxamide, N-[3-(2-cyclobutylcyclopropyl)-2-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-40-5 HCAPLUS CN H-Pyrcole3-carboxamide, N-[3-(2-cyclobutylcyclopropyl)-2-thienyl]-4-(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-41-6 HCAPLUS
CN IH-Pyrrole-3-carboxamide, N-[3-(2-cyclopentylcyclopropyl)-2-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) cyclopentylcyclopropyl)-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-45-0 HCAPLUS
CN H-Fyrrole-3-carboxamide, N-[3-(2-cyclopentylcyclopropyl)-2-thienyl]-2-fluoro-1,4-dimethyl- (SCI) (CA INDEX NAME)



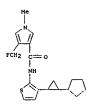
RN 688324-47-2 HCAPLUS
CN 1H-Pyrcle-3-carboxamide, 2-chloro-N-[3-(2-cyclopentylcyclopropyl)-2thienyl]-1,4-dimethyl- (9C1) (CA INDEX NAME)

RN 688324-48-3 HCAPLUS
CN lH-Pyrclola-3-carboxamide, N-[3-(2-cyclohexylcyclopropyl}-2-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-42-7 HCAPLUS
CN lH-Pyrrole-3-carboxamide, N-[3-[2-cyclopentylcyclopropyl)-2-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-43-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cyclopentylcyclopropyl)-2-thienyl]-4(fluoromethyl)-1-methyl- (SCI) (CA INDEX NAME)



RN 688324-44-9 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-(3-(2-

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-49-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cyclohexylcyclopropyl)-2-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-50-7 HCAPLUS
CN H-Pyrrole-3-carboxamide, N-(3-(2-cyclohexylcyclopropyl)-2-thienyl]-4(fluoromethyl)-1-methyl- (9C1) (CA INDEX NAME)

RN 688324-51-8 HCAPLUS
CN HH-Pyrrola-3-carboxamide, 4-(chlorodifluoromethyl)-N-[3-(2-cyclohexylcyclopropyl)-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-52-9 HCAPLUS CN H-Pyrrole-3-cerboxamide, N-[3-(3-cyclohexyl-2,2-difluorocyclopropyl)-2thienyl)-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

LB ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-53-0 HCAPLUS CN HH-Pyrrole-3-carboxamide, N-[3-(2-cyclohexylcyclopropyl)-2-thienyl]-2fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-54-1 HCAPLUS CN H-Pyrrole-3-carboxamide, 2-chloro-N-(3-(2-cyclohexylcyclopropyl)-2thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-55-2 HCAPLUS

(N 1H-Pyrrole-3-carboxmide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-56-3 HCAPLUS

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-60-9 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-2fluoro-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-61-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 688324-62-1 HCAPLUS
CN IH-Pyrrole-3-carboxamide, N-[3-(2-cyclooctylcyclopropyl)-2-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-63-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-cyclooctylcyclopropyl)-2-thienyl]-4(difluoromethyl)-1-methyl- [9CI) (CA INDEX NAME)

Page 1530/08/2005

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrrole-3-carboxamide, N-{3-(2-cycloheptylcyclopropyl)-2-thienyl}-1ethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-57-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-58-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-4(fluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-59-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(chlorodifluoromethyl)-N-[3-(2-cycloheptylcyclopropyl)-2-thienyl]-2-fluoro-1-methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-64-3 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-n-[3-(2-phenylcyclopropyl)-2-thienyl]-4(trifluoromethyl)- (9C1) (CA INDEX NAME)

RN 688324-65-4 HCAPLUS CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-(2-phenylcyclopropyl)-2-thienyl]- (9CI) (CA INDEX NAME)

RN 688324-66-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(fluoromethyl)-1-methyl-N-(3-(2-phenylcyclopropyl)-2-thienyl]- (SCI) (CA INDEX NAME)

RN 688324-67-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-fluoro-1, 4-dimethyl-N-[3-(2-phenylcyclopropyl)-2-thienyll-(9C1) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 688324-68-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-{3-(2-phenylcyclopropyl)-2-thienyl]- (9CI) (CA INDEX NAME)

RN 688324-69-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-(4-fluorophenyl)cyclopropyl]-2-thienyl]1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-70-1 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 4-(difluoromethyl)-N-[3-[2-(4-fluorophenyl)cyclopropyl]-2-thienyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 688324-71-2 HCAPLUS

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 688324-75-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-[2-(2-thienyl)cyclopropyl]-2thienyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-76-7 HCAPLUS

NH-Pyrrole-3-carboxamide, 1-methyl-N-[3-[2-(3-thienyl)cyclopropyl]-2-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-77-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-(2-furanyl)cyclopropyl)-2-thienyl]-1methyl-4-(trifluoromethyl)- [9CI) (CA INDEX NAME)

RN 688324-78-9 HCAPLUS

Page 1630/08/2005

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-(4-chlorophenyl)cyclopropyl]-2-thienyl)1-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-72-3 HCAPLUS
CN 1H-Pyrcole-3-carboxamide, N-{3-{2-(4-chlorophenyl)cyclopropyl}-2-thienyl}4-(difluoromethyl)-1-methyl- (9C1) (CA INDEX NAME)

RN 688324-73-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-[4-bromophenyl]cyclopropyl]-2-thienyl]-1methyl-4-(trifluoromethyl)- (9C1) (CA INDEX NAME)

RN 688324-74-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[3-{2-{4-bromophenyl}cyclopropyl}-2-thienyl}-4(difluoromethyl)-1-methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrrole-3-carboxamide, N-[3-[2-(3-furanyl)cyclopropyl]-2-thienyl]-1methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-79-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-methyl-N-[3-(1'-methyl[1,1'-bicyclopropyl]-2-y1)-2-thienyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 688324-80-3 HCAPLUS
CN 1H-Pytrole-3-carboxamide, 4-(difluoromethyl)-1-methyl-N-[3-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-2-thienyl]- (9C1) (CA INDEX NAME)

RN 688324-81-4 HCAPLUS
CN IM-Pyrcole-3-carboxamide, 2-fluoro-1,4-dimethyl-N-(3-(1'-methyl[1,1'-bicyclopropyl]-2-yl)-2-thienyl]- (9CI) (CA IMDEX NAME)

ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

688324-82-5 HCAPLUS |H-Pyrrole-3-carboxamide, 2-chloro-1,4-dimethyl-N-(3-(1'-methyl(1,1'-bicyclopropyli-2-yl)-2-thienyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 683815-41-0 HCAPLUS HH-Pytrole-2-carboxamide, 4-(acetylamino)-N-[4-[[[5-([[3-(dimethylamino)propyl]amino]carbonyl]-1-methyl-1H-pytrol-3-yl]amino]carbonyl]-5-methyl-2-thienyl]-1-methyl- (9CI) (CA INDEX NAME)

IT 683815-68-1P G83815-69-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation, antimicrobial and antifungal activities of heterocyclic amino acid trimers as distamycin analogs with enhanced lipophilicity)
683815-69-1P
BRAPEUS
HP-Pyrrole-2-carboxamide, N-[4-[[[5-[[3-(dimethylamino)propyl]amino]carbon nyl]-1-methyl-1H-pyrcol-3-yl]amino]carbonyl]-5-methyl-2-thienyl]-1-methyl-4-nitro- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 05 Mar 2004 Forty-eight heterocyclic amino acid trimers, analogs of distamycin, with a number of features that enhance lipophilicity are described. They contain alkyl or cycloalkyl groups larger than methyl: some are N-terminated by acetamide or methoxybenzamide and are C-terminated by dimethylaminopropyl or aliphatic heterocyclic aminopropyl substituents. The ability of these compds. to bind principally to AT tracts of DNA has been evaluated using capillary zone electrophoresis. Significant antimicrobial activity against key organisms such as MRSA and Candida albicans is shown by several compds., especially those containing a thiazole. Moreover, these ds.

Compds.

compds.

compds.

have low toxicity with respect to several mammalian cell lines.

ACCESSION NUMBER: 2004:178994 HCAPLUS

DOUMENT NUMBER: 140:375474

AUTHOR(S): Synthesis and Antimicrobial Activity

Khalef, Abedawn 1: Waigh, Roger D.: Drummond, Allan
J.: Pringle, Breffni: McGroarty, lan: Skellern, Graham
G.: Suckling, Colin J.

CORPORATE SOURCE: Department of Pure Applied Chemistry and Department of
Pharmaceutical Sciences, University of Strathclyde,
Glasgow, Gl lXL, UK

SOURCE: Journal of Medicinal Chemistry (2004), 47(8),
2133-2156

CODEN: JMCMAR: ISSN: 0022-2623

American Chemical Society

DOUMENT TYPE: Journal

DOCUMENT TYPE: LANGUAGE: IT 683815-40-

MENT TYPE: Journal
UNGE: English
683815-40-9P 683815-41-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(preparation, antimicrobial and antifungal activities of heterocyclic amino
acid trimers as distamycin analogs with enhanced lipophilicity)
683815-40-9 HCAPLUS
HI-Pyrrole-2-carboxamide, N-(4-[[[5-[[3-(dimethylamino)propyl]amino]carbo
nyl]-1-methyl-IH-pyrrol-3-yl]amino]carbonyl]-5-methyl-2-thienyl]-4(formylamino)-1-methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 6 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 02 Sep 2003

AB The eight novel polyamides: PyPyPyBDp, ImPyPpPyDp,
 ImPyPyDp, PyImImBDp, ImImImBDp, PyPyImBDp,
 ImPyImpDp, and PyImPyBDp (Py = N-methylpyrrole, Im =
 N-methylping) Amount of the properties of the sense of the sens

140:128669
Fragmentation mechanisms of polyamides containing
N-methylpyrrole and N-methylimidazole by electrospray
ionization tandem mass spectrometry
Yuan, Gu; Tang, Feili; Zhu, Chang Jin; Liu, Yan; Zhao,

AUTHOR (S):

CORPORATE SOURCE:

Yu Fen
Department of Chemical Biology, The Key Laboratory of
Bioorganic Chemistry and Molecular Engineering,
Ministry of Education, College of Chemistry, Peking
University, Beijing, 100871, Peop. Rep. China
Rapid Communications in Mass Spectrometry (2003),
17(17), 2015-2018
CODEN: RCMSPE: ISSN: 0951-4198
John Wiley & Sons Ltd.
Journal

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: Journal

MENT TYPE: Journal
UAGE: English
648928-24-9P 648928-25-0P 648928-29-4P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical
process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(fragmentation mechanisms of polyamidae containing methylpytrole and
methylimidazole by electrospray ionization tandem mass spectrometry)
648928-24-9 HCAPLUS
1H-Pytrole-2-carboxamide, N-[5-[[[3-[[3-(dimethylaminolpropyl]amino]-3oxopropyl]amino[carbonyl]-1-methyl-1H-pytrol-2-yl]-1-methyl-1-F1H-pytrol-2-yl)carbonyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-B



648928-25-0 HCAPLUS

IN-Imidazole-2-carboxamide, N-[5-[[[5-[[3-[(3-(dimethylamino)propyl]amino]-3-oxopropyl]amino]carbonyl]-1-methyl-1Hpyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl- (9CI) (CA
INDEX NAME)

L8 ANSWER 6 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

648928-29-4 HCAPLUS
1H-Imidazole-2-carboxamide, N-[3-[[3-(dimethylamino)propyl]amino]-3cxopropyl]-1-methyl-5-[[[1-methyl-1H-pyrrol-2yl)carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-B

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN (Continued)
9J, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 200108187 A5 20020313 AU 2001-80187 20010827
PRIORITY APPLN. INFO.: W0 2001-JP7321 A 20000828

OTHER SOURCE(S): MARPAT 136:232201

IT 403617-43-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)

(Dreparation of cyclic amine derivs. as CCR3 antagonists)

(1)2-Pyrrolidinedicarboxamide, N2-(3-cyano-2-thienyl)-N1-((3-exo)-8-((6-fluoro-2-naphthalenyl)methyl]-8-azabicyclo[3.2.1]oct-3-yl)-, (2S)- (9CI)

(CA INDEX NAME)

403478-55-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclic amine deriva. as CCR3 antagonists)
403478-55-7 HCAPUS
1-Pyrrolidinecarboxylic acid, 2-[(3-cyano-2-thienyl)amino)carbonyl}-,
9H-fluoren-9-ylmethyl ester, (2S)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Page 1830/08/2005

ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 08 Mar 2002

AB The title compds. I [ring A = (un)substituted heterocyclic ring, etc.; X = bond, O. Co, etc.; ring B = 01, etc.; ring V3 = hydrocarbon ring, etc.; X = CH, N: Y = CO, etc.; R21, R22 = H, halo, etc.; T1 = (CH2)n: n = 0 - 2; ring D = (un)substituted aryl, etc.] are prepared In an in vitro test (for CCR3 antagonism) using cells, compds. of this invention showed IC50 values of 0.001 μM to 0.45 μM.

ACCESSION NUMBER: 2002:171853 HCAPLUS
DOCUMENT NUMBER: 136:232201
TITLE: Preparation of cyclic amine derivatives as CCR3 antagonists

Moribitra, Koichiro: Inami, Hiroshi; Kubota, Hirokazu; Yokoyama, Kazuhiro: Morokata, Tatsuaki; Takeuchi, Makoto: Takahashi, Toshiya; Kaneko, Masayuki; Imaoka, Takayuki; Torii, Yuichi; Iura, Yosuke

PATENT ASSIGNEE(S): PATENT TYPE: Patent Information:

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

PAT	ENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE	
						-											
WO	2002	0183	35		A1		2002	0307	1	WO 2	001-	JP73	21		2	0010	827
	W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		co,	CR.	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GÉ,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE.	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	ΜX,	MZ,	NO,	ΝZ,	PH,	PL,
		PT,	RO,	RU,	SD,	SÈ,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT.	ΤZ,	UA,	UG,
		US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
		DF.	DK	PQ	FT	FD	GB	CB	TE	TT	1.11	MC	NT.	PT	SE:	TR	BF.

L8 ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 28 Dec 2001

AB The title compds. [I; R1, R2 = H, halo, aryl, etc.; or R1 and R2 taken together form (CH2)m(NR4)n(CH2)p (wherein m, p = 1-3; n = 0-1; m + n + p = 3-5; R4 = H, alkyl); R3 = alkyl, alkenyl, aryl, etc.], useful in the treatment of diseases caused by and/or associated with an altered protein kinase activity such as cancer, cell proliferative disorders, Alzheimer's disease, viral infections, auto-immune diseases and neurodegenerative disorders (no data given), were prepared Thus, amidation of 2-aminon-3-carbomyl-4, 5, 6, 7-tetrahydrobenzo[b]thiophene with phenylacetic acid afforded I [R1R2 = (CH2)4; R3 = CH2PH].

ACCESSION NUMMER: 2001-9335593 HCAPLUS hCAP

LANGUAGE: PATENT INFORMATION: 1

PA:	TENT I	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE.	
						-									-		
WO	2001	0982	90		A2		2001	1227	1	WO 2	001-	EP67	63		2	0010	614
WO	2001	0982	90		A3		2002	0516									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ВŻ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,
		RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,
		UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM		
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
US	6414	013			В1		2002	0702	1	US 2	000-	5965	50		2	0000	619
CA	2414	085			AA		2001	1227		CA 2	001-	2414	085		2	0010	614
AU	2001	0857	45		A5		2002	0102		AU 2	001-	8574	5		2	0010	614
EP	1294	707			A2		2003	0326		EP 2	001-	9649	83		2	0010	614
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,

ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

383380-90-3 HCAPLUS

2-Pyrrolidinecarboxamide, 1-acetyl-N-[3-(aminocarbonyl)-5-(1-phenylethyl)-2-thienyl]-4-hydroxy- (9CI) (CA INDEX NAME)

383381-04-2 HCAPLUS
1H-Indole-2-carboxamide, N-[3-(aminocarbonyl)-5-(1-phenylethyl)-2-thienyl]1-methyl- (9CI) (CA INDEX NAME)

383381-05-3 HCAPLUS
1H-Indole-3-carboxamide, N-{3-(aminocarbonyl)-5-(1-phenylethyl)-2-thienyl]1-methyl- (SCI) (CA INDEX NAME)

Page 1930/08/2005

L8 ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2004501146 22004015 JP 2002-504246

PRIORITY APPLN. INFO.: US 2000-596550
WO 2001-EP6763 (Continued) 20010614 A 20000619 W 20010614 OTHER SOURCE(S): MARPAT 136:69729
IT 383379-42-09 383379-77-9P 383380-21-0P 383380-90-3P 383381-04-2P 383381-05-3P RL: PAC (Pharmacological activity): SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
[preparation of thiophene-3-carboxamides as kinase inhibitors]
383379-42-8 HCAPEUS
HI-Pyrrole-2-carboxamide, N-[3-(aminocarbonyl)-4,5,6,7tetrahydrobenzo[b]thien-2-yl]-1-methyl- (9CI) (CA INDEX NAME)

383379-77-9 HCAPLUS 2-Pyrrolidinecarboxamide, N-[3-(aminocarboxyl)-5-(1-methylethyl)-2-thienyl]-1-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

383380-21-0 HCAPLUS 2-Pyrrolidinecarboxamide, 1-acety1-N-[3-{aminocarbony1}-5-pheny1-2-thieny1]- (SCI) (CA INDEX NAME)

L8 ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

ANSWER 9 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 26 Sep 2000

AB N-linked five-membered heteroaryls were obtained by conversion of 2-carboxy-heteroarenes I (Y = OH, R = H, Me, SiMe3, X = S, Se, O) into N-(2-heteroaryl)-1-methylpyrrole-2-carboxamides II. The procedure is based on a simple thermal rearrangement of thiophene or selenophene carbonyl azides I (Y = N3) in neat 1-methylpyrrole at 90°.

ACCESSION NUMBER: 2000:673727 HCAPLUS

DOCUMENT NUMBER: 134:100944

A convenient and efficient conversion of 2-carboxyheteroarenes into and N-(2-thienyl and 2-selenophenyl) 1-methylpyrrole-2-carboxamides

Danielli, Filippor Zanirato, Paolo

Dip. di Chim. Organica, 'A. Mangini', Univ. di
Bologna, Bologna, 40136, Italy

ARKIVOC (online computer file) (2000), 1(1), '67-72

CODEN: AKVCFI

URL: http://www.arkat.org/arkat/journal/Issuel/ARK0000
09/ms9.pdf

PUBLISHER: ARKAT Foundation

OCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

CTHER SOURCE(S): CASREACT 134:100944

CASREACT 134:100944

319447-91-1P 319447-95-5P 319447-97-7P 319447-99-9P

1-methyl-N-2-thienyl- (9CI) (CA INDEX NAME)

ŔŃ 319447-95-5 HCAPLUS

ANSWER 10 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 15 Sep 2000

A new aromatic pair, 2-hydroxy-6-methoxybenzamide/1-methylpyrrole at the terminal position of hairpin polyamides has been designed for distinguishing T-A from A-T base pairs and both from G-C/C-G in the minor groove of DNA. Four eight-ring hairpin polyamides with benzamide (Bz), 2-hydroxybenzamide (Hb-1), 2-hydroxy-6-methylbenzamide (Hb-2), and 2-hydroxy-6-methylbenzamide (Hb-3) at the N-terminal position were synthesized. The equilibrium ciation

association

consts. (Ka) were determined at four DNA sites which differ at a single common consts. (Ka) were determined at four DNA sites which differ at a single common consts. (Ka) were the sequences of "THTACA-3" (N = T, A, G, C). Quant. DNAse I footprint titration expts. reveal that (Hb-3) PypyPy-(R)HZNy-TmPyPyPy-R)-Dp (4) bound the sequences 5"-TTTACA-3" and 5"-TTTACA-3" with high affinity; Ka = 2.6 + 1010 M-1 and Ka = 8.4 + 109 M-1, resp., a 3-fold specificity for T vs. A was found. Importantly, the sequences 5"-TCTACA-3" and 5"-TCTACA-3" are bound with 50 and 200 times lower affinity, revealing an overall specificity of Hb-3/Py of T > A » G > C. These results expand the repertoire of sequences targetable by hairpin polyamides.

ACCESSION NUMBER: 134:26617

DOCUMENT NUMBER: 134:26617

134:26617

Hydroxybenzamide/Byrrole Pair Distinguishes T-A
from A·T Base Pairs in the Minor Groove of DNA
Ellervik, Ulf: Wang, Clay C. C.: Dervan, Peter B.
Division of Chemistry and Chemical Engineering,
California Institute of Technology, Pasadena, CA,
91125, USA
Journal of the American Chemical Society (2000),
122(39), 9354-9360
CODEN: JACSAT: ISSN: 0002-7863
American Chemical Society AUTHOR(S): CORPORATE SOURCE:

SOURCE:

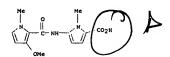
American Chemical Society Journal PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

312299-02-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

RL: RCT (Reactant); SPN (Synthetic preparation); rntr (rrepaired); rock (Reactant or reagent) (Reactant or reagent) (Polyamides containing hydroxybenzamide/pyrrole pair distinguish T-A from A-T base pairs in minor groove of DNA) 312299-02-8 HCAPLUS |
H-Pyrrole-2-carboxylic acid, 5-[((3-methoxy-1-methyl-1H-pyrrol-2-yl)carbonyl]amino]-1-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1H-Pyrrole-2-carboxamide, N-2-furanyl-1-methyl- (9CI) (CA INDEX NAME)

319447-97-7 HCAPLUS 1H-Pyrcole-2-carboxamide, 1-methyl-N-(5-methyl-2-thienyl)- (9CI) (CA INDEX NAME)

319447-99-9 HCAPLUS

xamide, 1-methyl-N-[5-(trimethylsilyl)-2-threnyl)- (9CI) (CA INDEX NAME)

SiMe

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 13 Jul 2000

AB Head-to-head linked dimers of heterocyclic amino acids were prepared to investigate their affinity and selectivity in binding to the minor groove of DNA. The selection of targets for synthesis was led by computer based design. Several novel dicarboxylic acid linkers including indoles, phenanthrenes, a fluorenone, and a bisbenzothiophene were included. Anal. of binding to DNA by footprinting showed high affinity for compds. derived from 2,7-dihydrophenanthrenedicarboxylic acid and a predominate selectivity for AT rich regions containing at least four AT pairs but with the ability to span up to two CG base pairs.

ACCESSION NUMBER: 2000:471732 HCAPLUS

DOCUMENT NUMBER: 133:281718

DOCUMENT NUMBER:

TITLE:

AUTHOR (S):

133:281718
The synthesis of some head to head linked DNA minor groove binders
Khalaf, A. I.; Pitt, A. R.; Scobie, M.; Suckling, C.
J.; Urwin, J.; Waigh, R. D.; Fishleigh, R. V.; Young,
S. C.; Wylie, W. A.
Department of Pure and Applied Chemistry, University
of Strathclyde, Glasgow, Gl IXL, UK
Tetrahedron (2000), 56(29), 5225-5239
CODEN: TETRAB; ISSN: 0040-4020
Elsevier Science Ltd.
Journal
English CORPORATE SOURCE:

SOURCE:

PUBLISHER DOCUMENT TYPE: LANGUAGE:

English CASREACT 133:281718

OTHER SOURCE (S) :

Z99974-91-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of head-to-head linked heterocyclic amino acid dimers with binding affinity to minor groove of DNA)
299974-91-7 HCAPLUS
HN-Pyrrole-2-carboxamide, N-[5-[[(3-(dimethylamino)propyl]amino]carbonyl]-2-thienyl]-1-methyl-4-nitro- (9CI) (CA INDEX NAME)

44

REFERENCE COUNT:

THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 12 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 12 May 2000

B A process of synthesizing a bicyclo compound (I) is described. Proline (II) is reacted with diphenylphosphinic chloride to activate the carboxylic acid group, and then reacted with methanesulfonyl chloride to produce ester (III) which is then reacted with a group II metal sulfide source in water to produce I.

CCESSION NUMBER: 2000:307143 HCAPLUS

DOCUMENT NUMBER: TITLE:

2000:307143 HCAPLUS
132:321855
Process for synthesizing carbapenem side chain intermediates
Brands, Karel M. J., Williams, John M.; Dolling, Ul. H.; Jobson, Ronald B.; Davies, Antony J.; Cottrell, Ian F.; Cameron, Mark; Ashwood, Michael S. Merck and Co., Inc., USA
U.S., 13 pp., Division of U.S. Ser. No. 106,297.
CODEN: USXXAM
Patent
English INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: FAMILY ACC. NUM. COUNT:

PATENT NO. KIND DATE APPLICATION NO. DATE US 1999-334398 US 1998-106297 US 1998-106297 US 1997-52032P US 6060607 US 6063931 20000509 19990616 PRIORITY APPLN. INFO.: A3 P

OTHER SOURCE(S): IT 266337-28-4P CASREACT 132:321855; MARPAT 132:321855

RL: SPN (Synthetic preparation); PREP (Preparation) (process for synthesizing carbapenem side chain intermediates) 266337-28-4 HCAPLUS

1-Pyrrolidinecarboxylic acid, 2-{[(5-carboxy-2-thienyl)amino]carbonyl]-4-hydroxy-, 1-{1,1-dimethylethyl} ester, {2S,4S}- (9CI) {CA INDEX NAME}

ANSWER 13 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 07 Apr 2000 A synthetic combinatorial library of 10,000 components mostly containing atic

a synthetic tembranetrial fibrary of 10,000 Components makely Containing amino acids was screened for inhibition of DNase I cleavage at two ARE sequences. Ten amino acid building blocks were used to generate the library in which the N and C terminal residues were fixed and the four central positions of the peptide ligands were varied. The DNase I footprinting assay led, after deconvolution through sublibrary synthesis, to the identification of CGL-6382 as an ARE-selective minor groove binder containing a N-terminal nicotinic acid motif adjacent to a N-methyllmidazole unit and three N-methylpyrrole units coupled to a C-terminal argininamide residue. The optimized ligand CGL-6382 was found to recognize a 5'-GC(A/T)(A/T) motif within the two cloned androgen receptors responsive elements. The discovery of CGL-6382 as an ARE-selective ligand augurs well for the use of the DNase I footprinting methodol to identify sequence-specific DNA recognition ligands from large mixts. of small mols. (c) 2000 Academic Press.
SSION NUMBER: 2000:224933 HCAPLUS

2000:224933 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: TITLE: 133:68541

AUTHOR (S):

CORPORATE SOURCE:

133:68-41
An ARE-selective DNA minor groove binder from a combinatorial approach
Hamy, Francois; Albrecht, Genevieve; Florsheimer, Andreas; Bailly, Christian
Department of Oncology, Novartis Pharma Research, Basel, CH-4002, Switz.
Biochemical and Biophysical Research Communications (2000), 270(2), 393-399
CODEN: BBRCA9: ISSN: 0006-291X
Academic Press
Journal SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: IT 278788-95-

278788-95-72

RE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(an ARE-selective DNA minor groove binder from a combinatorial

approach) 278788-95-7 HCAPLUS

2/8788-95-7 HCAPLUS
3-Pyridinecarboxamide, N-[2-{{(5-{{(5-{{(5-{{(5-{{(15-{{(15-{{(15-{{(15-{{(15-{{(15-{17-}
yter)} 13-methyl-1H-pyrrol-2-y}] amino]carbonyl}-1-methyl-1H-pyrrol-3-y}] amino]carbonyl}-1-methyl-1H-pyrrol-3-y] amino]carbonyl}-1-methyl-1H-imidazol-4-yl]- (9CI) (CA INDEX NAME)

ANSWER 12 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN lute stereochemistry. (Continued)

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 41 KCAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 01 Dec 1999
B The synthesis, biol. activity, and DNA-binding properties of a series of
four pyrrolo[2,1-c][1,4]benzodiazepine (PBD) hybrids containing polypyrrole
side chains are described and structure-activity relationships examined To
investigate sequence selectivity and stability of drug/DNA complexes,
DNase I footprinting and arrested polymerase chain reaction (PCR) were
performed on human c-myc oncogene, estrogen receptor gene, and human
immunodeficiency virus type I long terminal repeat (HIV-I UTR) gene
sequences. The antiproliferative activity of the hybrids was tested in
vitro on human myeloid leukemia KS52 and T-lymphoid Jurkat cell lines and
compared to antiproliferative effects of the natural product distamycin A
1, its tetrapyrrole homolog, DC 81, and a PBD ester. The new hybrids
exhibit different DNA-binding activity with respect to both distamycin A 1
and the parent PBD. In addition, a direct relationship was found between the
number of pyrrole rings present in the hybrids and the stability of drug/DNA
complexes. With respect to antiproliferative effects, it was found that
the increase of in vitro antiproliferative effects, i.e., the hybrid with 4
pyrroles is more active than the other ones both against KS62 and Jurkat
cell lines.

ACCESSION NUMBER:

1999:758546 HCAPLUS

DOCUMENT NUMBER:

1999:758546 HCAPLUS

DOCUMENT NUMBER:

1999:758546 HCAPLUS

Synthesia, in Vitro Antiproliferative Activity, and
DNA-Binding Properties of Hybrid Molecules Containing
Pyrrolo[2,1-c]11,41benzodiazeoine and

increase of in vitro antiproliferative effects, i.e., the hybrid with 4 pyrroles is more active than the other ones both against K562 and Jurkat cell lines.

ACCESSION NUMBER: 1999:758546 HCAPLUS
DOCUMENT NUMBER: 132:137361

TITLE: Synthesis, in Vitro Antiproliferative Activity, and DNA-Binding Properties of Hybrid Molecules Containing Pyrrolo[2,1-c][1,4]benzodiazepine and Minor-Groove-Binding Olioppyrrole Carriers

AUTHOR(S): Baraldi, Pier Giovanni; Balboni, Gianfranco; Cacciari, Barbara; Guiotto, Andrea; Manfredini, Stefano; Romagnoli, Romeo; Spalluto, Giampiero; Thurston, David E.; Howard, Philip W.; Bianchi, Nicoletta; Rutigliano, Cristina; Mischiati, Carlo; Gambari, Roberto

Oipartimento di Scienze Farmaceutiche e Dipartimento di Biochimica e Biologia Molecolare, Universita di Ferrara, Ferrara, 44100, Italy

SOURCE: Journal of Medicinal Chemistry (1999), 42(25), 5131-5141

CODEN: JMCMAR; ISSN: 0022-2623

American Chemical Society

DOUMENT TYPE: Journal

LANGUMGE: JSSO 49-78-70-99

RL: BAC (Biological activity or effector, except adverse); BSU (Biological atudy, unclassified); PEP (Physical, engineering or chemical process); SNO (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(Process)

(Preparation, antiproliferative activity, and DNA-binding pyrrolobenzodiazepines containing oligopyrrole carriers)

RN 256949-69-6 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-5-[([1-methyl-5-[[1-c][1],4]benzodiazepin-8-yl)oxylpropyl)amino]-1H-pyrrol-2-yl]carbonyl]amino]-, monohydrochloride (SCI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

• HCl

PAGE 1-B

256949-62-9

235949-62-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(preparation, antiproliferative activity, and DNA-binding
pyrrolobenzodiazepines containing oligopyrrole carriers)
256949-62-9 HCAPLUS
1H-Pyrrole-2-carboxamide, N-[5-[[[3-amino-3-iminopropyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-5-[[[3-amino-1-methyl-1H-pyrrol-2-yl]-5-[[0-amino-1-methyl-1H-pyrrol-2-yl]-1-methyl-1-methyl-1H-pyrrol-2-yl]-1-methyl-1, dihydrochloride (9CI) (CA INDEX NAME)

ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

• HC1

PAGE 1-B

256949-70-9 HCAPLUS

1H-Pyrrole-2-carboxamide, N-[5-[[[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-5-[[[1-axc-3-[[(1aS)-2,3,5,11a-tetrahydro-7-methoxy-5-oxo-1H-pyrrolo[2,1-c](1,4]benzodiazepin-8-yl]oxylpropyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-, monohydrochloride

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

PAGE 1-A

●2 HC1

PAGE 1-B

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236949-61-8

RE: RCT (Reactant): RACT (Reactant or reagent)
(preparation, antiproliferative activity, and DNA-binding
pyrrolobenzodiazepines containing oligopyrrole carriers)
236949-61-8 HCAPLUS
1H-Pyrrole-2-carboxamide, N-[5-[[(3-amino-3-iminopropy)]amino]carbonyl]-1methyl-1H-pyrrol-3-yl]-5-[[(5-amino-1-methyl-1H-pyrrol-2yl)carbonyl]amino]-1-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

256949-65-2P 256949-66-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, antiproliferative activity, and DNA-binding pyrrolobenzodiazepines containing oligopyrrole carriers)

ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 256949-65-2 MCAPLUS | H-Pyrrolo[2,1-c][1,4]benzodiazepine-10(5H)-carboxylic acid, B-[3-[[5-[[5-[[5-[[5-[13-amino-3-miniopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[-3-oxopropoxyl]-2,3,11,1la-tetrahydro-1l-hydroxy-7-methoxy-5-oxo-, 2,2,2-trichloroethyl ester, monohydrochloride, (115,11aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

HC1

PAGE 1-B

256949-66-3 HCAPLUS

1H-Pyrrolo[2,1-c][1,4]benzodiazepine-l0[5H]-carboxylic acid,

8-[3-[[5-[[5-[[5-([5-([6-k]]-amino-3-iminopropy]) amino]carbonyl]-1-methyl
1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1
methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]-3
coxpropoxyl-2,3,1l,1la-tettahydro-1l-hydroxy-7-methoxy-5-oxo-,

2,2,2-trichloroethyl ester, monohydrochloride, (118,11a5)- (9CI) (CA

TNDFX NAME) INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 26 Aug 1998 L8 ED GI

$$\begin{array}{c|c} \text{CH}_{2}\text{O} & & \text{CH}_{2}\text{NHCO} \\ \text{Ph} & & \text{CO} & \text{Ph} \\ \end{array}$$

AB The title compds., e.g. I [Rl represents optionally substituted aralkyl, etc.: Z represents optionally alkylated nitrogen, etc.; Xl represents CHZNHCO, etc.: X2 represents phenylene, etc.; X3 represents a single bond, etc.: Y2 represents optionally substituted aryl, etc.: and B represents oxygen, etc.], are prepared In an in vitro test for cPLA2 inhibition, the title compound II showed ICSO of 0.17 mM.

ACCESSION NUMBER: 1998:543071 HCAPLUS
DOCUMENT NUMBER: 129:161558
TITLE: Preparation and formulation of thiazolidinedione derivatives as phospholiage A2 inhibitors.

129:161558
Preparation and formulation of thiazolidinedione derivatives as phospholipase A2 inhibitors Seno, Kaorus Ohtani, Mitsuski: Watanabe, Fumihiko Shionogi 4 Co., Ltd., Japan PCT Int. Appl., 178 pp.
CODEN: PIXXD2 INVENTOR (5): PATENT ASSIGNEE(S): SOURCE:

LANGUAGE: PATENT Japanese FAHILY ACC. NUN. COUNT: 1
PATENT INFORMATION:

PAT	PENT .	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE	
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WO	9833	797			A1		1998	0806	1	WO 1	998-	JP30	7		1	9980	127
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		KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,
		NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	UA,
		UG,	US,	UZ,	VN,	YU,	ZW,	AM,	AZ,	BY,	KG,	ΚŹ,	MD,	RU,	TJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	DE,	DK,	ES,	FI,
		FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	BJ,	CF,	CG,	CI,	CM,
		GΑ,	GN,	ML,	MR,	NE,	SN,	TD,	TG								
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CA	2277	947			AA		1998	0806	1	CA 1	998-	2277	947	•	1	9980	127
CA	2277	947			C		2004	0921									

Page 2330/08/2005

ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

REFERENCE COUNT:

39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L	8 ANS	WER	15 0	F 41	HC	APLU	s c	OPYR:	IGHT	2005	A	cs	on	STN		(Co	ntin	ued)		
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		9903				Ä		1999						3706				9990		
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		9907				A		2000		M	v	199	٥	7061			1	9990	1729	
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OTHER SOURCE(S): MARPAT 129:161558

IT 211297-31-3P 211297-34-6P 211298-04-3P
211298-06-5P
RL: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): THU (Therapeutic use): BIOL (Biological study): PREP (Preparation): USES (Uses)
(preparation of thiazolidinedione derivs. as phospholipase A2 inhibitors)
RN 211297-31-3 HOAPLUS
CN 2-Pyrrolidinecarboxamide, 4-([1,1'-biphenyl]-2-ylmethoxy)-1-[2-(4-fluorobenzoyl]-bnzoyl]-N-[5-(4-0xo-2-thioxo-5-thiazolidinylidene)methyl]2-thienyl]-, (2S, 4R)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

211297-34-6 HCAPLUS
2-Pyrrolidinecarboxamide, 4-{[1,1'-biphenyl]-2-ylmethoxy}-N-[5-{(2,4-dioxo-5-thiazolidinylidene)methyl}-2-thienyl]-1-[2-{4-methylbenzoyl]benzoyl}-, (25,4R)- (9CI) (CA INDEX NAME)

L8 ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Absolute stereochemistry. Double bond geometry unknown. (Continued)

211298-04-3 HCAPLUS 2-Pyrrolidinecerboxamide, 4-{{[1,1'-biphenyl]-2-ylmethyl}thio}-N-{5-{(2,4-dioxo-5-thiazolidinylidene)methyl}-2-thienyl}-1-{2-(4-fluorobenzoyl)benzoyl}-, (2S,4R}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
1-Pyrrolidinecarboxylic acid, 4-[(1,1'-biphenyl]-2-plmethoxy)-2-[[[5-[(2,4-dioxo-5-thiazolidinylidene)methyl]-2-thienyl]amino]carbonyl]-,
1,1-dimethylethyl ester, (2S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

211298-06-5 HCAPLUS
2-Pyrrolidinecarboxamide, 4-[([1,1'-bipheny1]-2-ylmethy1)thio]-1-[2-(4-fluorobenzoy1)bnzoy1]-N-[5-[(4-oxo-2-thioxo-5-thiazolidinylidene)methy1]-2-thieny1]-, (2S, 4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

IT 211298-68-9P 211298-69-0P

RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of thiazolidinedione derivs. as phospholipase A2 inhibitors) 211298-68-9 HCAPLUS

tyleparation of thiazolidinedione derivs. as phospholipase A2 inhibitor 211298-68-9 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-{{1,1'-biphenyl}-2-ylmethoxy}-2-[[(5-formyl-2-thienyl)amino]carbonyl]-, 1,1-dimethylethyl ester, (2S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

211298-69-0 HCAPLUS

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 20 Aug 1997

A new upper limit of binding site size is defined for the hairpin polyamide-DNA motif. Ten-ring hairpin polyamides containing pyrrole (Py) and imidazole (Im) amino acids were designed for recognition of seven base pair (bp) sequences in the minor groove of DNA. The DNA binding properties of two polyamides, ImpPypPyPy-TmPPyPyPyPy-Dp, and ImImPyPyPy-y-ImPyPyPyPy-B-Dp were analyzed by footprinting and affinity cleavage on a DNA fragment containing the resp. match sites 5'-TGTARCA-3' and 5'-TGGARCA-3'. Quant. footprint titrns. demonstrate that ImpPyPyPy-y-ImPyPyPyPy-B-Dp binds the 7-Dp match sequence 5'-TGTARCA-3' with an equilibrium association constant (Ka) of Ka = 1.2 + 1010 M-1 and 18-fold specificity vs. the single base pair mismatch sequence 5'-TGGARCA-3'. ImImPyPyPyPy-D-Dp by a single amino acid substitution and binds its match 5'-TGGARCA-3' site with Ka = 3.6 + 109 M-1 and 300-fold specificity vs. its corresponding single base pair mismatch sequence 5'-TGTARCA-1'. Ten-ring hairpin polyamides have binding affinities similar to those of eight-ring hairpin polyamides. These results indicate that the affinity of hairpin binding ceases to increase as the length of the polyamide subunits increases beyond four rings, analogous to the behavior of unlinked subunits. Therefore, recognition of seven base pairs by a ten-ring hairpin polyamide most likely represents an upper limit to the effective targetable site size of the hairpin polyamide-DNA motif.

ACCESSION NUMBER: 1997:528757 HCAPLUS
DOCUMENT NUMBER: 1975:528757 HCAPLUS
COUMENT NUMBER: 17:216506
Recognition of Seven Base Pair Sequences in the Minor Groove of DNA by Ten-Ring Pyrrole-Imidazole Polyamide Hairpins

TITLE:

Recognition of Seven Base Pair Sequences in the Minor Groove of DNA by Ten-Ring Pyrrole-Imidazole Polyamide Hairpins

AUTHOR(S):

Turner, James M.; Baird, Eldon E.; Dervan, Peter B.

CORPORATE SOURCE:

Division of Chemistry and Chemical Engineering,

California Institute of Technology, Pasadena, CA,

S1125, USA

SOURCE:

Journal of the American Chemical Society (1997),

119(33), 7636-7644

CODEN: JACSAT: ISSN: 0002-7863

PUBLISHER:

American Chemical Society

Journal

LANGUAGE:

BPR (Biological process): BSU (Biological study, unclassified); CAT

(Catalyst use): SPN (Synthetic preparation); BIOL (Biological study): PREP

(Preparation): PROC (Process): USES (Uses)

(preparation): PROC (Process): USES (Uses)

RN 194857-41-5 HCAPELUS

CN Iron, (2,3,4,5-tetradehydro-1-methyl-4-[([1-methyl-4-[(1-methyl-4-[([1-methyl-4-[(1-methyl-4-

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

PAGE 1-C

ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

PAGE 1-C

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

PAGE 2-B

(Continued)

PAGE 2-C

194857-42-6 HCAPLUS

Iron, (2, 3, 4, 5-tetradehydro-1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-[{[1-methyl-4-{[[1-methyl-4-{[1-methyl-4-{[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[]]]]]]]]}}} y||carbonyl|amino|-1H-pyrrol-2-yl|carbonyl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myohyoryl|amino|-1-myo

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

PAGE 2-B

PAGE 2-C

194057-40-4P 194057-49-3P 194057-50-6P RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(Process) ation of and recognition of seven base pair sequences in the minor groove of DNA by ten-ring pyrole-imidazole polyamide heirpins)

194857-40-4 HAPRUS

194857-4 HAPRUS

194857-

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-C

- (CH2) 3 - NHMe

ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

194857-50-6 HCAPLUS

B-Alaninamide, 2,3,4,5-tetradehydro-1-methyl-4-[{{1-methyl-4-[-methyl-4-[-methy

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

 $\label{eq:continuous} $$194857-49-3$$$ HCAPLUS $$\beta-Alaninamide, 2,3,4,5-tetradehydro-1-methyl-4-[[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-[1-methyl-4-methyl-4-methyl-4-methyl-4-methyl-4-methyl-4-methyl-4-methyl-4-methyl-4-methyl-4-[1-methyl-4-[1-methyl-4-me$

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-C

LB ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

194857-46-0DP, conjugates with Pam resin 194857-47-1P
194857-48-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of and recognition of seven base pair sequences in the minor
groove of DNA by ten-ring pyrrole-imidazole polyamide hairpins)
194857-46-0 HCAPLUS
B-Rlanine, 2, 3, 4, 5-tetradehydro-1-methyl-4-[[(1-methyl-4-[[(1-methyl-4-[([1-methyl-4-[([1-methyl-4-[([1-methyl-4-[([1-methyl-4-[([1-methyl-4-[([1-methyl-4-[([1-methyl-4-[(1-me

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

PAGE 1-C

(Continued)

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

L8 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

PAGE 1-C

-- (CH2) 3-NH- (CH2) 3-NH2

PAGE 2-A

194857-48-2 HCAPLUS

LB ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-C

- (CH2) 3-NH- (CH2) 3-NH2

ANSWER 17 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 27 Apr 1996

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is directed to novel cyclopropylpyrroloindole-oligopeptide compds. Which are useful as anticancer agents. The novel cyclopropylpyrroloindole-oligopeptide compds. However, the property of the pro

123:148U
Cyclopropapyrroloindole-oligopeptide anticancer agents
Lown, J. William: Wang, Yuqiang; Luo, Weide
Symphar Laboratories, Inc., Can.
U.S., 17 pp.
CODEN: USXXAM

PATENT ASSIGNEE (S) : SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PA	TENT	NO.			KIN	D	DATE			APP	LICAT	ION	NO.		D.	ATE		
						-									-			
US	5502	068			А		1996	0326		US	1995-	3813	55		1	9950	131	
CA	2210	093			AA		1996	8080		CA	1996-	2210	093		1	9960	131	
WO	9623	497			A1		1996	8080		WO	1996~	US72	7		1	9960	131	
	W:	AL,	AM,	AT,	AU,	AZ,	BB,	BG,	BR,	BY	, CA,	CH,	CN,	CZ,	DE,	DK,	EE,	
		ES,	FI,	GB,	GE,	ΗU,	ÍS,	JP,	KE,	KG	, KP,	KR,	KZ,	LK,	LR,	LS,	LT,	
		LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO	, NZ,	PL,	PT,	RO,	RU,	SD,	SE,	
		SG,	SI															
	RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH	, DE,	DK,	ES,	FR,	GB,	GR,	IE,	
		IT,	LU,	MC,	NL,	PT,	SΕ,	BF,	BJ,	CF	, CG,	CI,	CM,	GA,	GN,	ML,	MR,	NE
AU	9649	643			Al		1996	0821		ΑU	1996-	4964	3		1	9960	131	
ΑU	6980	01			B2		1998	1022										
EP	8003	90			A1		1997	1015		ĒР	1996-	9061	76		1	9960	131	
EP	8003	90			B1		2002	1204										
	R:	AT,	ΒE,	CH,	DΕ,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	MC,	PT,	ΙE

Page 2830/08/2005

ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 2-A

ANSWER 17 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN
JP 11500427 T2 19990112 JP 1996-523576
AT 228837 E 20021215 AT 1996-906176
US 1995-381355
WO 1996-US727 (Continued) 19960131 19960131 A 19950131 W 19960131 PRIORITY APPLN. INFO.: OTHER SOURCE(S): IT 177177-56-9 MARPAT 125:11480

Nice To Product

ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 23 Dec 1995

AB Novel aminoalkyl substituted indolocarbazoles I (R = Q1 (n = 1, 2, 3), HN(CH2)3NMe2, etc.] were prepared from staurosporine aglycon and characterized with respect to inhibition of protein kinases C and A. In both series, potent and selective PKC inhibitors could be identified. Structure activity relationships are discussed.

ACCESSION NUMBER: 1995:1002243 HCAPLUS

DOCUMENT NUMBER: 124:175641

TITLE: Novel substituted indolocarbazoles as potent and selective inhibitors of protein kinase C

AUTHOR(S): Xie, Guojian; Nagata, Hiroyuki: Tamaoki, Tatsuya; Lown, J. William

CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Alberta, T6G 2G2, Can.
Bioorganic 4 Medicinal Chemistry Letters (1995), 5(23), 2841-4

CODDE: BMCLE8; ISSN: 0960-894X

FUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 17317-98-17 173917-99-2P

RLi BAC (Biological activity or effector, except adverse); BSU (Biologica

173917-98-1p 173917-99-2p
RL: BRC [Biological activity or effector, except adverse]: BSU [Biological study, unclassified]: SPN [Synthetic preparation]: BIOL (Biological study): PREP [Preparation]
(preparation and protein kinase inhibitory activity of indolocarbazoles)
173917-98-1 HCAPLUS
H-Pyrrole-2-carboxylic acid, 1-methyl-5-[{[1-methyl-5-{[1-oxo-3-(5,6,7,13-tetrahydro-7-oxo-12H-indolo[2,3-a]pyrrolo[3,4-c]carbazol-12yl]propyl]amino]-H-pyrrol-2-yl]carbonyl]amino]-, methyl ester [9CI] (CA INDEX NAME)

L8 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

173917-95-9 173917-96-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and protein kinase inhibitory activity of indolocarbazoles)
173917-95-8 HCAPLUS
HR-Pyrrole-2-carboxylic acid, 5-[[(5-amino-1-methyl-1H-pyrrol-2yllcarbonyllamino]-1-methyl-, methyl eater (9CI) (CA INDEX NAME)

L8 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

173917-99-2 HCAPLUS

1H-Pyrrole-2-carboxylic acid, 1-methyl-5-[[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[[1-methyl-5-[1-methyl-5

L8 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

$$\begin{array}{c|c} & & & & & \\ & & & & \\$$

173917-96-9 HCAPLUS
1H-Pyrrole-2-carboxylic acid, 5-{[[5-{['(5-amino-1-methyl-1H-pyrrol-2-yl)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-, methyl ester (9C1) (CA INDEX NAME)

$$\begin{picture}(20,0) \put(0,0){\line(1,0){100}} \put(0,0){\line(1,0){100$$

ANSWER 19 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 14 Dec 1995

AB Title compds. [I; Rl = H, halo, alkyl, alkoxy, etc.; R2 = (acyl)alkyl, acyl, CH:CHCO2H, etc.; R3 = H, alkyl, CH2Ph; R4 = SH, SnR, SeN, SenR, etc.; R = H, alkyl, (heterolaryl, I in which R4 = bond, etc.; R4R5 = S, Se; R5R6 = bond; R6 = H; n = 1-3] were prepared 2Hus, 1-methyl-2-indolinone was treated with P2S5 and the product condensed with PhNCO to give, after oxidation, title compound II which had ICSO of 3-4µM against growth factor mediated mitogenesis in vitro.

ACCESSION NUMBER: 1955:982654 HCAPLUS

DOCUMENT NUMBER: 124:175826

TITLE: Preparation of 2-indolyldisulfides and analogs as protein tyrosine kinase inhibitors and antitumor agents

INVENTOR(S): Dobrusin, Ellen M.; Showalter, Howard D. H.; Denny, William A.; Palmer, Brian D.; Rewcastle, Gordon W.; Tercel, Moans: Thompson, Andrew M.

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

U.S., 53 pp. Cont.-in-part of U.S. Ser. No. 926, 015, abandoned.

CODEN: USXAM

DOCUMENT TYPE: Patent

INVENTOR (S):

DOCUMENT TYPE: FAMILY ACC. NUM. COUNT: 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5464861	А	19951107	US 1993-94792	19930809
HU 71553	A2	19951228	HU 1995-341	19930802
CZ 283965	В6	19980715	CZ 1995-288	19930802
NZ 255194	Α	20000128	NZ 1993-255194	19930802
US 5556874	A	19960917	US 1995-438616	19950510
PRIORITY APPLN. INFO.:			US 1992-926015 B	2 19920806
			US 1993-94792 A	3 19930809

OTHER SOURCE(S): IT 156136-37-7P MARPAT 124:175826

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

EN ANSWER 20 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

Entered STN: 10 Jan 1995

B A series of 3 -substituted 2,2'-dithiobis(lH-indoles) were synthesized and evaluated for their ability to inhibit the tyrosine kinase activity of both the epidermal growth factor receptor [EGFR] and the nonreceptor pp60v-src tyrosine kinase, to extend the available structure-activity relationships for this series. The majority of the compds. were prepared either by reaction of 2-chloro-1-methylindole-3-carbonyl chloride with amines, followed by thlomethylation, demethylation, and oxidative dimerization, or by reaction of isocyanates with the anion of 1-methyl-2-indolinathione followed by dimerization. Overall, inhibitory activity is retained by analogs having a wide variety of side chains. A series of 3-carboxamide analogs had moderate to good activity against isolated EGFR (ICS0s 1-20 µM), with monealkyl substitution of the carboxamide being optimal. Polar side chains were generally less effective than lipophilic ones, with benzyl being particularly effective. However, N,N-disubstitution was the most effective pattern for inhibition of pp60v-src. A variety of substituted N-phenylcarboxamides had lower activity against EGFR than the parent derivative, and a N-thienylcarboxamide also had low activity. A series of 3-ketones, including Me, Ph, and furyl derivs., showed moderate activity against the pp60v-src kinase, but were less effective against EGFR. The mechanism of inhibition of both kinases by these drugs was shown to be noncompetitive with respect to both AFP and peptide substrate. Selected compds. inhibited the growth of Swiss 373 cells with IC50s in the low micromolar range and inhibition of both kinases by these drugs was shown to be noncompetitive with respect to both AFP and peptide substrate. Selected compds. inhibited the growth of Swiss 373 cells with IC50s in the low micromolar range and inhibition before-mediated intracellular tyrosine phosphorylation in the same cell line. Thiol inhibits the effects of the compds. S

DOCUMENT NUMBER:

1995:283548 HCAPIUS
123:248
Tyrosine Kinase Inhibitors. 4. Structure-Activity
Relationships among N- and 3-Substituted
2,2'-Dithiobis(1H-indolea) for in vitro Inhibition of
Receptor and Nonreceptor Protein Tyrosine Kinases
Palmer, Brian D.; Rewcastle, Gordon W.; Thompson,
Andrew M.; Boyd, Maruta; Showalter, H. D. Hollis:
Sercel, Anthony D.; Fry, David W.; Kreker, Alan J.;
Denny, William A.
School of Medicine, University of Auckland, Auckland,
92019, N. Z.
JOURNAI Of Medicinal Chemistry (1995), 38(1), 58-67
CODEN: JMCMAR; ISSN: 0022-2623
American Chemical Society
Journal

AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

156136-37-7P

155136-37-79
RL: BAC (Biological activity or effector, except adverse): BSU (Biological atudy, unclassified): SPN (Synthetic preparation); BIOL (Biological study): PREP: (Preparation) (astructure-activity relationships among dithiobisindoles for inhibition of receptor and nonreceptor protein tyrosine kinases)
156136-37-7 HCAPLUS
1H-Indole-3-carboxamide, 2,2'-dithiobis[1-methyl-N-2-thienyl- (9CI) (CA INDEX NAME)

ANSWER 19 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 2-indolyldisulfides and analogs as protein tyrosine kinase inhibitors and antitumor agents) 156136-37-7 HCAPLUS
1H-Indole-3-carboxamide, 2,2'-dithiobis[1-methyl-N-2-thienyl- (9CI) (CAINDEY NAME)

L8 ANSWER 20 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

EN ANSWER 21 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN
Entered STN: 17 Nov 1994
AB In the present study, the authors have investigated the effect of unprecedented chemical modifications introduced in the distanycin mol., with the aim of assessing their ability to interfere with sequence-specific DNA-protein interactions in vitro. By using an electrophoretic mobility shift assay, the authors have been able to identify novel distanycin analogs with improved displacing abilities on the binding of octamer nuclear factors to their target DNA sequence. While variations in the number of pyrrole rings and/or reversion of an internal amide bond result in distamycin-like compds. with identical or very simular properties, the reversion of the formamido into a carboxyamido group or its seplacement with the charged formimidoyl moiety significantly improves the ability of the resulting novel distamycin derive, to compete with OCT-1 (octamer 1 nuclear factor) for its target DNA sequence. Tissue-specific octamer-dependent in vitro transcription is similarly affected by these chemical modifications, suggesting that the ability of distamycins to bind octamer sequences has a direct influence on the functional state of octamer recontaining promoters. These data represent an initial, successful attempt Tartionalize the design of DNA binding drugs, using distamycins as a model.

ACCLESSION NOMER: 1995:199500 HCAPLUS
DOCUMENT NUMBER: 122:45671

as a model.
ACCESSION NUMBER: 1995:199500 HCAPLUS
DOCUMENT NUMBER: 122:45671

TITLE: Distamycin analogs with improved sequence-specific DNA binding activities

AUTHOR(S): Ciucci, Alessandra; Periotto, Giordana; Mischiati, Carlo; Gambari, Roberto; Animati, Fabio; Lombardi, Paolo; Natali, Pier Giorgio; Arcamone, Pederico; Giacomini, Patririo

CORPORATE SOURCE: Menarini Ricerche Sud, Italy
SOURCE: Biochemical Pharmacology (1994), 48(8), 1583-91

CODEN: BCPCA6; ISSN: 0006-2952

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal

IT 159565-63-6, MEN 10398 159565-64-7, MEN 10557

RL: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified); PRP (Properties): THU (Therapeutic use): BIOL (Biological study): USES (Uses)

(distamycin analogs with improved sequence-specific DNA binding activities)

RN 159565-63-6 HCAPLUS

RN 159565-63-6 HCAPLUS

RN 159565-63-6 HCAPLUS

RN 159565-63-6 HCAPLUS

RN 1597crole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[4-(formylamino)-1-methyl-1H-pyrrol-2-yl]-x monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 10 Dec 1994

AB Title compds. I (A = (substituted) Ph or thienyl: R1 = MeCH(OH), MeCHF, MoCH2: R2 = H, C1-4 alkyl: R3, R4 = H, halo, NC, C1-4 alkyl, O2N, HO, MOZC, C1-4 alkoxy, F3C, etc.:x = c1-6 alkanediyl interrupted by O, S(0)x wherein x = 0-2, RSNCO wherein X = B, C1-4 alkyl) or a salt or in vivo hydrolyasble ester, are prepared To allyl (IR,SS,6S,8R,2'S,4'S)-2-(1-allyloxycarbonyl-2-(3(Ea-llyloxycarbonyl-1-ethenyl)phenylcarbamoyl)pyrrolid din-4-ylthio)-6-(1-hydroxyethyl)-1-methylcarbapenem-3-carboxylate (preparation given) and Maldrum's acid in DMF and THF was added (PhB)+PdF dollowed by Na 2-ethylnexanoate to give the title compound (IR,SS,6S,8R,2'S,4'S)-2-(2-(3(E2-carboxy-1-ethenyl)phenylcarbamoyl)pyrrolidin-4-ylthio)-6-(1-hydroxyethyl)-1-methylcarbapenem-3-carboxylcacid, di-Na salt (II). In vitro against S. aureus the min. inhibitory concentration of II was 0.13 µg/mL ws. 2.0 µg/mL of cettriaxone. Pharmaceutical formulations comprising I are given.

ACCESSION NUMBER: 1994:680467 HCAPLUS

DOCUMENT NUMBER: 121:280467

TITLE: Preparation of antibiotic carbapenem compounds

121:280467
Preparation of antibiotic carbapenem compounds
Betts, Michael John; Davies, Gareth Morse; Jung,
Frederic Henri
Zeneca Ltd., UK; Zeneca Pharma S.A.
Eur. Pat. Appl., 27 pp.
CODEN: EPEXXDW
Patent
Fredith TITLE: INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PAT	ENT	NO				KINE)	DATE			API	PLICA	40 I T	NO.		D	ATE		
																	-			
	EP	590	885				A1		1994	0406		EΡ	1993	-307	551		1	9930	923	
	EP	590	885				Bl		2000	0315										
		R:	A:	r,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	R, IE	, 17	, LI,	LU,	MC,	NL,	PT,	SE
	CA	210	614	1			AA		1994	0329		CA	1993	-210	6141		1	9930	914	
	US	552	779	1			A		1996	0618		US	1993	-123	1998		1	9930	921	
	AT	190	615				E		2000	0415		AT	1993	-307	551		1	9930	923	
	ES	214	444	6			T3		2000	0616		ES	1993	-307	551		1	9930	923	
	JP	062	118	60			A2		1994	0802		JP	1993	-241	519		1	9930	928	
RIO	RITY	' AP	PLN	. :	INFO	. :						EΡ	1992	-402	648		A 1	9920	928	
THE	R SC	URC	E (S	: (MARE	TA	121:	2804	67									
Т	154	308	-86-	81	154	308-	87-91	15	8743	-30-7	72									
				-																

154308-86-8P 154308-87-9P 188743-3U-rr
158743-31-8P 158743-32-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of carbapenem antibiotics)
154308-86-8 HCAPLUS
154308-86-8 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[{[5-{2propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (25-cis)- (9CI) (CA INDEX NAME)

Page 3130/08/2005

ANSWER 21 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

159565-64-7 HCAPLUS
1H-Pyrrole-2,4-dicarboxamide, N4-[4-[{[4-{aminocarbonyl}-1-methyl-1H-pyrrol-2-yl]-n2-{3-amino-3-iminopropyl}-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L8 ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) Absolute stereochemistry.

154308-87-9 HCAPLUS

19430-07-9 mcRu33 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[(5-carboxy-2-thienyl)amino[carbonyl]-, 1-[(4-nitrophenyl)methyl] ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

158743-30-7 HCAPLUS

1337333 . nernos
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[5[[(carboxymethyl)amino]carbonyl]-2-thienyl]amino]carbonyl]-,
1-[(4-nitrophenyl]methyl] ester, (23-cis)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

158743-31-8 HCAPLUS 13843-31-8 (CAPLUS
1-Pyrrolidinecarboxylic acid, 2-[[[5-[[(carboxymethyl)amino]carbonyl]-2thienyl]amino]carbonyl]-4-mercapto-, 1-[(4-nitrophenyl)methyl] ester,
(23-cia)- [9C1) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

158743-32-9 HCAPLUS
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[5-[[5[[(carboxymethyl) smino]carbonyl]-2-thienyl]amino]carbonyl]-1-[((4nitrophenyl]methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4methyl-7-oxo-, 2-[(4-nitrophenyl]methyl] ester, [4R[3(35*,55*),4a,58,68[R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

LB ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Absolute stereochemistry. (Continued)

155481-44-0 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-mercapto-2-[[[5-[(2-propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

156631-45-7 HCAPLUS

130631-43-7 RAPLUS
4-Thia-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid,
6-[1-[(1,1-dimethylethyl) dimethylsilyl]oxy]ethyl]-3-[[1-[(4nitrophenyl)methoxyl]carbonyl]-5-[[[5-[(2-propenyloxy)carbonyl]-2thienyl]mmino[carbonyl]-3-pyrrolidinyl]thio]-7-oxo-, 2-propenyl ester,
[58-[3]35-5,55-),5a,6u[8^)]]- (9c1) (CA INDEX NAME)

Absolute stereochemistry.

Page 3230/08/2005

ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 03 Sep 1994

Title compds. I (R1 = MeCHMe, MeCHF, HOCH2: R2 = H, C1-4 alkyl: Z = HO2C, HO3S, tetrazol-5-yl, C1-4alkyl-50ZNHCO: A = (substituted)Ph or thienyl) a pharmaceutically acceptable salt or in vivo hydrolyzable ester thereof, are prepared 2-Thiophenecarboxylic acid was nitated to give the 4-nitro derivative, reduced ti the 4-amino derivative converted to the (25, 45)-1-(4-nitrobenzylcarbonyl)-2-(2-carboxy-4-thienylcarbomyol)pyrrolidin-4-ylthioacetate which in in 4 steps was converted to (5R, 6S, 8R, 2'S, 4'S)-1 (R1 = MeCHOH, R2 = H, A = 4-thienyl, Z = 2-HO2C) which had a min. inhibitory concentration of 0.5 mg/mL against Enterobacter cloacea 108 vs 32 mg/L of ceftriaxone. Pharmaceutical formulations comprising I are given.

SSION NUMBER: 1994:508368 HCAPLUS
MEMT NUMBER: 121:108368

EE: Preparation of antibiotic pyrrolidinylthiopenem

TITLE:

INVENTOR(S):

PATENT ASSIGNEE (S):

SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 592167	A1	19940413	EP 1993-307843	19931001
EP 592167	B1	19991222		
R: AT, BÉ, CH,	DE, DK	ES, FR,	GB, GR, IE, IT, LI, LU,	
CA 2106330	AA	19940408	CA 1993-2106330	19930916
AT 187968	E	20000115	AT 1993-307843	19931001
ES 2140445	т3	20000301	ES 1993-307843	19931001
JP 06211871	A2	19940802	JP 1993-250437	19931006
US 5538962	A	19960723	US 1993-132256	19931006
ORITY APPLN. INFO.:			EP 1992-402733	A 19921007
ER SOURCE(S):	MARPAT	121:10836	8	

ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

156631-46-8 HCAPLUS

136531-40-8 HCAPLUS
4-Thia-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid,
6-(1-hydroxyethyl)-3-[[1-[[(4-nitrophenyl)methoxy|carbonyl]-5-[[[5-[(2-propenyloxy)carbonyl)-2-thienyl]aminolcarbonyl]-3-pyrcolidinyl]thio]-7-oxo-,
2-propenyl ester, [5R-[3(33*,55*),5α,6α(R*)]]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 03 Sep 1994
A simple 10-membered monocyclic 3-ene-1,5-diyne has been prepared tethered to a derivative of innetropsin. It is proposed that the attachment to this reactive diyne-ene to a moli which assocs. with B-DNA in the minor groove can enhance the potency of the diyne-ene as a DNA cleavage agent. The nature of the tether appears to be very important in the magnitude of this enhancement, based on two examples reported here. With a two-carbon tether, there is a small increase in DNA cleavage compared with the parent diyne-ene. However, a four-carbon tether, based on a crotonate linkage, shows almost a 2000-fold enhancement of the parent diyne-ene. DNA binding studies using CD measurements and ethidium bromide displacement show that the relative binding constant of the diyne-ene and the two versions tethered to netropsin parallel the DNA cleavage effectiveness.

ACCESSION NUMBER: 1994:495071 HCAPLUS
DOCUMENT NUMBER: 121:99071
TITLE: Simple Cyclic Enediyne to a Netropsin Analog Semmelhack, M. F.; Gallagher, J. J.; Ding, W.-d.; Krishnamurthy, G.; Babine, R.; Ellestad, G. A.

CORPORATE SOURCE: Semmelhack, M. F.; Gallagher, J. J.; Ding, W.-d.; Krishnamurthy, G.; Babine, R.; Ellestad, G. A.

DEPARTMENT of Chemistry, Princeton University, Princeton, NJ, 08544, USA

JOURNAI of Organic Chemistry (1994), 59(16), 4357-9

CODEN: JOCEAN; ISSN: 0022-3263

DOCUMENT TYPE: Journal of Organic Chemistry (1994), 59(16), 4357-9

CODEN: JOCEAN; ISSN: 0022-3263

DOCUMENT TYPE: Journal of Organic Chemistry (1994), 59(16), 4357-9

CODEN: JOCEAN; ISSN: 0022-3263

THAPPYROID-2-carboxamide, 4-amino-N-[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-1H-pyrrol-2-carboxamide, 4-amino-N-[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-1H-pyrrol-2-carboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CM 1

CM 156055-65-1

CM 15605

L8 ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued

ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 2 CRN 156055-64-0 CMF C14 H16 03 сн2-со2н 156055-69-5 HCAPLUS
2-Butenoic acid, 4-(4-cyclododecene-2,6-diyn-1-yloxy)-, compd. with
4-(13-amino-3-imino-1-oxopropyl)aminol-N-(5-[[(3-amino-3-iminopropyl)amino|carbonyl)-1-methyl-1H-pyrrol-2-yl]-1-methyl-1H-pyrrol-2-yl СМ 2 CRN 156055-67-3 CMF C16 H18 O3 о- сн2- сн== сн- со2н ANSWER 25 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 20 Aug 1994 AB Title compds. [I; Rl = H, halo, OH, alkyl, alkoxy, CO2H, etc.; l or 2 CRl
= N; R2 = (acyl)alkyl, CH:CKCO2H, alkylcarbabamoyl, acyl, etc.; R3 = H,
alkyl, CH2Ph; R4 = ZH, ZNX, ZNQ; R5 = H and R4R6 = S or Se; R5R6 = bond; Q = I in which R4 = Zn and R5R6 = bond; X = H, alkyl, CH2Ph, (hetero)aryl; 2
= S, Se; n = 0-3] were prepared Thus, l-methyl-2-indolinone was treated with P25S and the product treated with NaH and PhNCO to give indolinethionecarboxamide II which had IC50 of 2µM against epidermal growth factor mediated mitogenisis.

ACCESSION NUMBER: 1994:483305 NCAPLUS
DOCUMENT NUMBER: 12:83050
TITLE: 1994:483305 NCAPLUS
INVENTOR(S): 2018:3050
Preparation of 2-indolinethiones and related disulfides and seleno-analogs as protein tyrosine kinase inhibitors and antitumor agents
INVENTOR(S): Dobrusin, Ellen Myra; Showalter, Noward Daniel Hollis; Denny, William Alexander; Palmer, Brian Desmond; RewCasatle, Gordon William; Tercel, Moans; Thompson, Andrew Mark
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
PCT Int. Appl., 212 pp.
COODEN PIXXD2
DOCUMENT TYPE: Palmer, Foliab DOCUMENT TYPE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE A1 WO 9403427 19940217 WO 1993-US7272 19930802 WO 9403427 AI 19940217 WO 1993-US7272 19930802 W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE EP 654024 AI 19950524 EP 1993-918594 19930802 EP 654024 Al 19950524 EP 1993-918594 19930802 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, HU 71553 A2 19951228 HU 1995-341 19930802 JP 08503450 T2 19960926 JP 1993-519671 19930802 AU 672224 B2 19960926 AU 1993-47994 19930802 HU 71553 JP 08503450 AU 672224 AU 9347994 CZ 283965 NZ 255194 19940303 19980715 CZ 1995-288 NZ 1993-255194 RU 1995-108332 SK 1995-135 US 1992-926015 WO 1993-US7272 19930802 19930802 19930802 19930802 20000128 RU 2155187 20000827 20030701 SK 283413 PRIORITY APPLN, INFO.:

ANSWER 25 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

156136-37-7 HCAPLUS
HH-Indole-3-carboxamide, 2,2'-dithiobis[1-methyl-N-2-thienyl- (9CI) (CA
HDEX NAME)

L8 ANSWER 26 OF 41 HCAPLUS
JP 05508372 T2
JP 3313366 B2
AT 185140 E
ES 2136124 T3
CA 2108356 C
CN 1077957 A
CN 1036713 B
NO 9304264 A
FI 104075 B1
US 5515015 A
PRIORITY APPLN. INFO.: COPYRIGHT 2005 ACS on STN
19940922 JP 1993-516398
20020812
19991015 AT 1993-906740
20040120 CA 1993-106354
19931103 CA 1993-102800
19971217
19931125 NC 1993-4254
19991115 FI 1993-5245 (Continued) 19930324 AT 1993-906740 ES 1993-906740 CA 1993-2108356 CN 1993-102800 19930324 19930324 19930324 19930326 NO 1993-4264 FI 1993-5245 US 1993-142459 EP 1992-400836 EP 1992-402763 WO 1993-GB603 19931125 19931125 19960521 19920326

OTHER SOURCE(S): MARPAT 121:9029
IT 154308-86-89 155481-34-89 155481-36-09
155481-37-19 155481-38-29 155481-40-69
155481-41-79 155481-42-89 155481-43-99
155481-52-09 155481-53-19 155481-51-99
155481-52-09 355481-53-19 155549-68-79

155491-52-09 155491-53-1P 155549-48-TP
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(preparation and reaction of, in preparation of
carboxythienylcarbamoylpyrolidin
ylthiocarbapenemcarboxylates)
RN 154308-86-8 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[5-{[2propenyloxylcarbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl
ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155481-34-8 HCAPLUS 155481-34-8 RCAPLUS
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-[1-hydroxyethyl]-4-methyl-3-[[1-[[4-nitrophenyl]methoxy]carbonyl]-5-[[[4-[2-propenyloxy]carbonyl]-2-thienyl]amino[carbonyl]-3-pyrrolidinyl]thio]-7-oxo-, 2-propenyl ester, [4R-[3(35*,55*),4\alpha,5\beta,6\beta(R^*)]]-, compd. with N-ethyl-N-(1-methylethyl)-2-propanamine [1:1] [9CI] (CA INDEX NAME)

CM 1

CRN 155481-33-7 CMF C34 H36 N4 O11 S2

ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 09 Jul 1994

AB Title compds. I [R = (un)substituted carboxythienyl: Rl = CHMeOH, CHMeF, CH2OH: R2, R3 = R, alkyl] were prepared Thus, the carbapenem II was obtained from the diphenylphosphoryloxycarbapenem and the thiol, prepared from 2-thiophenecarboxylic acid and the protected mercaptopyrrolidinecarboxylic acid in 4 steps. 11 had min. inhibitory concus. against Staphylococcus aureus Oxford 0.125 and Escherichia coli DCO 0.008 µg/mL.

ACCESSION NUMBER: 1994:409029 HCAPLUS
DCOUMENT NUMBER: 121:9029

TITLE: Carbapenem derivatives as antibiotics and intermediates thereof

1994:409029 HCAPLUS
121:9029
Carbapenem derivatives as antibiotics and intermediates thereof
Jung, Frederic Henri
Zeneca Ltd., UK; Zeneca Pharma S. A.
PCT Int. Appl., 44 pp.
CODEN: PIXXD2
Patent

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA'	ENT :	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE		
						-									-			
WO	9319	070			A1		1993	0930		WO 1	993-	GB60	3		1	9930	324	
	W:	AT,	AU.	BB,	BG,	BR,	CA,	CH,	CZ,	DE,	DK,	ES,	FI,	GB,	HU,	JP,	KP,	
		KZ.	LK,	LU.	MG.	NL.	NO,	PL.	RO									
	RW:	AT.	BE.	CH.	DE.	DK.	ES,	FR.	GB,	GR,	IE.	IT.	LU,	MC,	NL,	PT,	SĒ,	
							CM,											
2A	9301	611			A		1993	0927		ZA 1	993-	1611			1	9930	305	
IL	1051	35			A1		2000	0131		IL 1	993-	1051	35		1	9930	323	
ΑU	9337	636			A1		1993	1021		AU 1	993-	3763	6		1	9930	324	
ΑU	6629	72			B2		1995	0921										
EP	5866	63			A1		1994	0316		EP I	993-	9067	40		1	9930	324	
£Ρ	5866	63			Bl		1999	0929										
	R:	AT.	BE.	CH.	DE.	DK,	ES.	FR.	GB,	GR,	IE,	IT.	LI,	LU,	MC.	NL,	PT,	s
****	CE 23	•			2.2		1004	A770			000-	2204				0020	224	

ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CM 2

CRN 7087-68-5 CMF C8 H19 N

155481-36-0 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[4-[(2-propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155481-37-1 HCAPLUS
1-Azabicyclo(3.2.0)hept-2-ene-2-carboxylic acid, 3-[[5-[[(3-carboxy-4,5,6,7-tertaph/drobenzo|b]thien-2-yl)amino|carbonyl]-1-[[(4-nitrophenyl)methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 2-(2-propenyl) ester, (4R-[3(35*,55*),4o,5\$,6.be
ta.(R*)]]-[9CI] (CA INDEX NAME)

L8 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) Absolute stereochemistry.

RN 155481-38-2 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[(3-carboxy-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]amino]carbonyl]-, 1-[(4-nitrophenyl)methyl]
ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 155481-40-6 HCAPLUS

CN 1-Azabicyclo(3.2.0)hept-2-ene-2-carboxylic acid, 3-[[5-[[(3-carboxy-4-methyl-2-thienyl)amino|carbonyl]-1-[[(4-nitrophenyl)methoxylcarbonyl]-3-pyrrolidinyl[thi0]-6-[1-hydroxyethyl]-4-methyl-7-oxo-, 2-(2-propenyl) ester, [4R-[3(35',55'),4a,5B,6B(R')]-, compd. with N-ethyl-N-(1-methylethyl)-2-propanamine [1:1) [9CI] (CA INDEX NAME)

CRN 155481-39-3 CMF C32 H34 N4 O11 S2

Absolute stereochemistry.

LB ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 155481-43-9 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethyl)-4-methyl-3-[[1-(14-nitrophenyl)methoxy]carbonyl]-5-[[[5-[(2-propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-3-pyrrolidinyl]thio]-7-oxo-(4-nitrophenyl)methyl ester, [4R-[3(35*,55*), 4α,5β,6β(R*)]]- [9C1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A

RN 155481-44-0 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-mercapto-2-[[[5-[(2-propenyloxy)carbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CM 2 CRN 7087-68-5 CMF C8 H19 N

Et | |-Pr-N-Pr-

RN 155481-41-7 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[3-(ethoxycarbonyl)-4-methyl-2-thienyl]smino)carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 155481-42-8 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[{3-carboxy-4-methyl-2-thienyl)amino[carbonyl]-4-mercapto-, 1-[{4-nitrophenyl)methyl] ester, (2S-cis)- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 155481-45-1 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[5-[[(5-carboxy-3-hydroxy-2-thienyl)amino]carbonyl]-1-[[[4-nitrophenyl]methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-[1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(48-).59-).4a, 5p, 66[R+)]]- [9CI] (CA INDEX NAME)

RN 155481-51-9 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[[3-(1,1-dimethylethoxy)-5[(1,1-dimethylethoxy)carbonyl]-2-thienyl]amino[carbonyl]-,
(4-nitrophenyl)methyl ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

155481-52-0 HCAPLUS
1-Pyrrolidinecarboxylic acid, 2-[[[5-carboxy-3-hydroxy-2-thienyl]amino]carbonyl]-4-mercapto-, 1-[(4-nitrophenyl)methyl] ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

155481-53-1 HCAPLUS
1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[5-[[5-carboxy-3-hydroxy-2-thienyl]amino]carbonyl]-1-[[(4-nitrophenyl]methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, <math>2-(2-propenyl) ester, $\{4R-[3(3s^*,5s^*),4\alpha,5\beta,6\beta(R^*)]\}-\{9CI\}$ (CA INDEX

Absolute stereochemistry.

ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 28 May 1994

Title compds. [I; R1 = 1-hydroxyethyl, 1-fluoroethyl, hydroxymethyl; R2, R3 = H, alkyl; R4 = Q1-Q3; Z = carboxy, sulfonic acid, sulfinic acid, phenylsulfonylcarbamoyl, alkoxycarbamoyl, alkanesulfonamido, cyanocarbamoyl, tetrazol-5-yl, 3-hydroxylsoxazol-4-yl, benzamidosulfonyl, etc.] were prepared Thus, (ZS,4S)-1-(4-nitrobenzyloxycarbonyl)-2-(3-sulfophenylcarbamoyl)pyrrolidin-4-ylthioscetate diisopropylethylamine salt (preparation given) was saponified with IN NaON and the resulting thiol was stirred with 4-nitrobenzyl (IR,5R,6S,8T)-6-(1-hydroxyethyl)-1-methyl-2-diphenylphosphoryloxycarbapenem-3-carboxylate (preparation given) in DMF aining

containing

disopropylethylamine and Bu3P to give a coupling product which was
hydrogenated in EtoAc/H2O/EtoN containing KHCO3 to give (18,55,65,87,2'5,4'5)2-[2-(3-sulfophenylcarbamoyl)pyrrolidin-4-ylthio]-6-(1-hydroxyethyl)-1methylcarbapenem-3-carboxylic acid dipotassium salt. This showed MIC's of
0.125 and 0.015 µg/mL against Staphylococcus aureus Oxford and
Escherichia coli DCO, resp.
ACCESSION NUMBER: 1994-269929 HCAPLUS
DOCUMENT NUMBER: 129:269929 HCAPLUS
TITLE: PROFESSION OXIGATION NUMBER: 129:269929 HCAPLUS

EP 562855 EP 562855 Al Bl 19930929 EP 1993-302296 19930325 GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
CA 1993-2091309
AT 1993-302296
ES 1993-302296
JP 1993-68076
US 1994-302394
EP 1992-400837
A 19920326
EP 1992-400839
A 19920326 EP 562855 B1
R: AT, BE, CH, DE,
CA 2091309 AA
T 179978 E
ES 2133358 T3
JP 06025244 A2 19990312 , ES, FR, 19930927 19990515 19990916 DK. 19940201 19961105 PRIORITY APPLN. INFO.:

Page 3630/08/2005

ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

155549-48-7 HCAPLUS 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, $3-[[5-[[(5-carboxy-3-hydroxy-2-thienyl)amino]acrbonyl]-1-[[(4-nitrophenyl)amino]acrbonyl]-3-pyrrolidinyl|thio|-6-(1-hydroxyethyl)-4-methyl-7-oxo-, [4R-[3(3S*,5S*),4<math>\alpha$,5 α ,6 β (R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN EP 1992-402700 US 1993-37171 (Continued) A 19921002 B1 19930326

OTHER SOURCE(S): MARPAT 120:269929
IT 154308-96-9P 154308-97-9P 154308-89-0P
154308-99-1P 154308-90-4P 154308-91-5P
154308-93-7P 154309-01-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for antibacterial)
RN 154308-86-8 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-([[5-(2-propenyloxylcarbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

154308-87-9 HCAPLUS
1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[(5-carboxy-2-thienyl)amino]carbonyl)-, 1-[(4-nitrophenyl)methyl] ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

154308-88-0 HCAPLUS
1-Pyrrolidinecerboxylic acid, 4-(acetylthio)-2-[[[5[(methylaulfonyl)amino]carbonyl]-2-thienyl]amino]carbonyl]-,
(4-nitrophenyl)methyl ester, (25-cis)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

O₂N SAC

RN 154308-89-1 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-mercapto-2-[[[5[[methylsulfonyl]amino]carbonyl]-2-thlenyl]amino]carbonyl]-,
(4-nitrophenyl)methyl ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 154308-90-4 HCAPLUS CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethy1)-4-methyl-3-[[5-[[15-[(methylsulfony1)amino]carbony1]-2-thienyl]amino]carbonyl]-1-[[[4-nitropheny])methoxy]carbonyl]-3-pyrrolidinyl]thio]-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(38*,58*), 4α , 5β , 6β (R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) CM 1

CRN 154308-92-6 CMF C36 H33 N7 O12 S2

Absolute stereochemistry.

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CM 2 CRN 7087-68-5 CMF C8 H19 N

Et

RN 154309-01-0 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[5-[(cyanoamino]carbonyl]-2thienyl]amino]carbonyl]-4-mercapto-, (4-nitrophenyl)methyl ester,
(2S-cis)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

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RN 154308-91-5 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 4-(acetylthio)-2-[[5-[(cyanoamino)carbonyl]-2-thienyl]amino]carbonyl]-, (4-nitrophenyl)methyl ester, (25-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

O_{2N} S_{Ac}

RN 154308-93-7 HCAPLUS
CN 1-Azabicyclo{3.2.0|hept-2-ene-2-carboxylic acid, 3-[[5-([[5-([cyanoamino)carbonyl]-2-thienyl]amino]carbonyl]-1-[[(4-nitrophenyl)methoxy]carbonyl]-3-pyrrolidinyl]thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-([3/35*,55*),40,56,68(R*)])-, compd. with
N-ethyl-N-(1-methylethyl)-2-propanamine (1:1) (9CI) (CA INDEX NAME)

L8 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

O_{2N} S_M

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 05 Mar 1994

R1R2NA (CH2) nX1 - CONH (CH2) 2C: NHNH2

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9313739	A2	19930722	WO 1993-EP2	19930104
WO 9313739	A3	19931125		
RW: AT, BE, CH,	DE, DK,	ES, FR, GB	, GR, IE, IT, LU, MC	, NL, PT, SE,
BF, BJ, CF,	CG, CI,	CM, GA, GN	, ML, MR, SN, TD, TO	;
AU 9333478	A1	19930803	AU 1993-33478	19930104
EP 623023	A1	19941109	EP 1993-902141	19930104
R: DE, ES, FR,	GB			
PRIORITY APPLN. INFO.:			IT 1992-MI21	A 19920110
			WO 1993-EP2	A 19930104
OTHER SOURCE(S):	MARPAT	120:107751		

150691-25-1P 150691-26-2P 150691-27-3P

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A - сн2- сн2с1 CH2- CH2C1

150691-27-3 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[4-[[4-[[14-[[14-[1] amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride
(9C1) (CA INDEX NAKE)

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS ON STN 150691-29-49 150691-29-59 150691-30-89 150691-33-19 150691-34-29 150691-35-39 150691-36-49 150691-40-09 (Continued)

130691-35-19 150691-36-49 150691-40-0P
RE: SPN (Synthetic preparation): PREP (Preparation)
(prepn. of, as anticancer and antivirus agent)
150691-25-1 HCAPEUS
1H-Pyrrole-2, 4-dicarboxamide, N2-{5-[[[5-[[(3-amino-3-iminopropyl)amino|carbonyl]-1-methyl-1H-pyrrol-3-yl]carbonyl]amino}-1-methyl-1H-pyrrol-3-yl]carbonyl]amino}-1-methyl-1H-pyrrol-3-yl]carbonyl]-1-methyl-,monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A сн2-сн2с3 сн₂- сн₂с1

150691-26-2 HCAPLUS
1H-Pyrrole-2, 4-dicatboxamide, N2-[5-[[{3-amino-3-iminopropyl}amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-N4-[4-[[4-[bis{2-chloroethyl}amino]benzoyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

150691-28-4 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropy))-N4-[4-[[[4-[[[4-[[i]s(2-chioroethy)]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-,
monohydrochloride (9CI) (CA INDEX NAME)

150691-29-5 HCAPLUS 1H-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropy))-N4-[4-[[[4-(bis(2-chloroethyl) amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-1, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

● HC1

150691-30-8 HCAPLUS
1H-Pyrrole-2,4-dicarboxamide, N2-{5-[[(3-amino-3-iminopropyl)amino]-1-methyl-1H-pyrrol-3-yl]-N4-[4-{bis(2-chlorocthyl)amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

150691-31-9 HCAPLUS
1H-Pyrrole-2,4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[4-[bis(2-chloroethyl)amino]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

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150691-34-2 HCAPLUS
1H-Pyrrole-2, 4-dlcarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[[4[(cyclopropylcarbonyl)amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

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● HC1

150691-35-3 HCAPLUS
1H-Pyrrole-2, (-dlcarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-{[[4-{[1-aziridinylcarbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

150691-33-1 HCAPLUS
1H-Pyrrole-Z, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-1-methyl-N4-[1-methyl-4-[(13-methyl-4-[(3-methyloxiranyl)carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]-, monohydrochloride (SCI) (CA INDEX NAME)

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ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

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● HC1

150691-36-4 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-{3-amino-3-iminopropyl}-N4-{4-[{[4-{{2-chlorol-0xov-2-propenyl}amino]-1-methyl-1H-pyrrol-2-yl}-arbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

RN 150691-40-0 HCAPLUS

methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

ΙT

150691-42-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of anticancer and antivirus agents)
150691-42-2 HCAPLUS
H-Pyrrole-2-carboxamide, 4-amino-N-[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-,

L8 ANSWER 29 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN
Entered STN: 08 Jan 1994
High resolution proton NMR techniques have been used to study the interaction
between the self-complementary Dickerson dodecamer (GCGCAATTCGCG)2 and
two distamycin nanlogs containing a retroinverted amide bond. The results
indicated that both analogs, although binding the Dickerson dodecamer less
strongly than distamycin, span the central AATT segment in the minor
groove in a similar fashion.

ACCESSION NUMBER: 1994:2947 HCAPLUS
DOCUMENT NUMBER: 1994:2947 PACPLUS
TITLE: PROFESSION NUMBER: 1994:2947 TITLE: PROFESSION NUMBER

DOCUMENT NUMBER: TITLE:

120:2947
Proton NMR studies of the interactions of two
distamycin analogs with the dodecamer d(CGCCAATTCGCG)2
Rosaria Conte, Maria; Fattorusso, Ernesto;
Gomez-Paloma, Luigi, Mayol, Luciano
Dip. Chim. Sostanze Nat., Univ. Napoli Federico,
Naples, I-80131, Italy
Bioorganic & Medicinal Chemistry Letters (1992),
2(10), 129-304
CODEN: BMCLE8; ISSN: 0960-894X AUTHOR (S):

CORPORATE SOURCE:

CODEN: BMCLE8; ISSN: 0960-894X

DOCUMENT TYPE: Journal
LANGUAGE: English

IT 143158-57-0
RL: PRP (Properties)
(double-atranded DNA dodecamer binding of, NMR study of)
RN 143158-57-0 HCAPLUS
CN 1H-Pyrrole-2, 4-dicarboxamide, NZ-(3-amino-3-iminopropyl)-N4-[4-([[4-([formylamino]-1-methyl-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN monohydrochloride (9CI) (CA INDEX NAME) (Continued)

● HC1

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 02 Oct 1993

AB The title compds. I [W = 0, S, NH; m, n = 1, 2, 3, 4; B, B1 = (CH2)pNR1R2, (CH2)qC(:NR3)NR4R5, B, B1 = (un)saturated (un)substituted (condensed) carbocyclic ring; (un)saturated (un)substituted heteromono- or -di-cycle; p = 2, 3, 4; R1, R2 = H, C1-6 alkyl; q = 1, 2, 3, 4; R3 = H, R4, R5 = H, C1-6 alkyl; R3R4 = CH:CH, CH2CH2, CH2CH2; R5 = H, C1-6 alkyl; land their pharmaceutically acceptable salts, useful as angiogenesis inhibitors (no data) and particularly in cancer therapy either alone or together with an antitumor agent, are prepd from anionethylpyrolecarboxemide derivs., e.g., II [W] = 0, S; X = leaving group) or their salts. Thus, e.g., II [W] = 0, S; X = leaving group) or their salts. Thus, specific salts are pyrolecarboxylimino)bis[i-(N, N-dimethylamino)asphthalene was prepared from 1,8-diaminonaphthalene and Ne 5-nitro-3-pyrrolecarboxylate in several of the control of

Derivatives of "Samino-I-methyl-3-pyrrolecarboxamadas angiogenesis inhibitors
Mongelli, Nicola: Biasoli, Giovanni; Paio, Alfredo;
Mariani, Mariangela
Farmitalia Carlo Erba S.r.l., Italy
Brit. UK Pat. Appl., 43 pp.
CODEN: BAXXDU

INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2260134	A1	19930407	GB 1991-21205	19911004
PRIORITY APPLN. INFO.:			GB 1991-21205	19911004
OTHER SOURCE(S):	MARPAT	119:139084		
TT 149621-64-7P				

149521-64-79
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[preparation and hydrogenation of)
149521-64-7 HCAPIUS
H-Pyrrole-3-carboxamide, N-[4-[[8-(dimethylamino)-1naphthalenyl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-5-nitro-

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (9CI) (CA INDEX NAME) (Continued)

149594-72-9P 149594-73-0P

149594-72-99 149594-73-0P
RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reaction of in synthesis of angiogenesis inhibitor)
149594-72-9 HCAPLUS
1,3,5-Naphthalenetrisulfonic acid, 8-[[[5-[[[5-amino-1-methyl-1H-pyrrol-3-yl]carbonyl]amino]-1-methyl-1H-pyrrol-3-yl]carbonyl]amino]-, trisodium
salt, monohydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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149594-73-0 HCAPLUS 1,3,5-Naphthalenetrisulfonic acid, 8-[[[1-methyl-5-[[(1-methyl-5-nitro-lH-pyrrol-3-yl]carbonyl]amino]-lH-pyrrol-3-yl]carbonyl]amino]-, trisodium salt (SCI) (CA INDEX NAME)

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

149594-76-3P 149621-63-6P 149621-70-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as angiogenesis inhibitor)
149594-76-3 HCAPLUS
1,3-Naphthalenedisulfonic acid, 7,7'-(carbonylbis(imino(1-methyl-1H-pyrrole-2,4-diyl)carbonyllmino(1-methyl-1H-pyrrole-2,4-diyl)carbonyllmino)|bis-, tetrapotassium salt (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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PAGE 2-A ●4 K

149621-63-6 HCAPLUS
1H-Pyrrole-3-carboxamide, 5,5'-(carbonyldiimino)bis[N-[4-[[8-(dimethylamino)-1-naphthalenyl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl- (9CI) (CA INDEX NAME)

149621-70-5 HCAPLUS
1,3,5-Naphthalenetrisulfonic acid, 8,8'-[carbonylbis(imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-

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ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN diyl)carbonylimino]}bis- (9CI) (CA INDEX NAME) (Continued)

PAGE 2-A 1 503H

149594-70-7P
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of, in synthesis of angiogenesis inhibitor)
149594-70-7 HCAPLUS
1H-Pyrrole-3-carboxamide, 5-amino-N-[4-[[8-(dimethylamino)-1-naphthalenyl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

●6 Na

149594-77-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in synthesis of angiogenesis inhibitor)
149594-77-4 HCAPLUS
1,3-Naphthalenedisulfonic acid, 7-[[[5-[[(5-amino-1-methyl-1H-pyrrol-3-yl]carbonyl]amino]-,monohydrochloride (9CI) (CA INDEX NAME)

• HC1

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ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

149594-71-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, protonation, and formulation of, as angiogenesis inhibitor)
149594-71-8 HCAPLUS
1,3,5-Naphthalenetrisulfonic acid, 8,8'-[carbonylbis[imino{1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino[]bis-, hexasodium salt (9CI) (CA INDEX NAME)

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

149621-72-7 149621-73-8 149621-74-9
149621-75-0 149621-76-1 149621-77-2
149621-75-0 149621-76-1 149621-80-7
149621-78-3 149621-79-1 149621-80-7
149621-81-1 149621-82-9 149621-80-7
149621-84-1 149621-85-2 149621-86-3
149621-84-1 149621-85-2 149621-86-3
149621-87-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(use of, as angiogenesis inhibitor)
149621-72-7 HCAPLUS
1H-Pyrrole-3-carboxamide, 5,5'-(carbonyldimino)bis(N-[4-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A сн₂- сн₂-

PAGE 2-B

— с— ин₂ || ин

149621-73-8 HCAPLUS Carbonimidic dihydrazide, 2,2'-bis[4-[[[4-[[[4-[[(3-amino-3-

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl)- (9CI) (CA INDEX NAME)

149621-74-9 HCAPLUS
1-Maphthalenesulfonic acid, 4,4'-{carbonylbis[imino{1-methyl-1H-pyrrole-2,4-diyl)carbonylimino{1-methyl-1H-pyrrole-2,4-diyl)carbonylimino}]bis-(9CI) (CA INDEX NAME)

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

149621-76-1 HCAPLUS
1,3-Maphthalenedisulfonic acid, 8,8'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]bis- (9CI) (CA INDEX NAME)

149621-77-2 HCAPLUS
1,7-Maphthalenedisulfonic acid, 4,4'-[cerbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino[bis- 19CI (CA INDEX NAME)

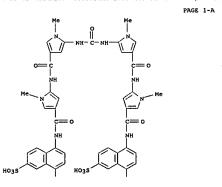
L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

149621-75-0 HCAPLUS
1-Maphthalenesulfonic acid, 8,8'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino[]bis-(9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)



PAGE 2-A | 503Н

149621-78-3 HCAPLUS
1,5-Maphthalenedisulfonic acid, 4,4'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino[]bis- (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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149621-79-4 HCAPLUS
1,3,6-Naphthalenetrisulfonic acid, 8,8'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl]carbonylimino(1-methyl-1H-pyrrole-2,4-diyl]carbonylimino]]bis- (9CI) (CA INDEX NAME)

ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

149621-81-8 HCAPLUS
1,3-Naphthalenedisulfonic acid, 6,6'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]]bis- (9CI) {CA INDEX NAME}

149621-82-9 HCAPLUS
1,7-Maphthalenedisulfonic acid, 3,3'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]bis-[9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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149621-80-7 HCAPLUS
1,5-Maphthalenedisulfonic acid, 7,7'-(carbonylbis(imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino)]bis- (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

149621-83-0 HCAPLUS 2,7-Maphthalenedisulfonic acid, 3,3'-[carbonylbis[imino[1-methyl-1H-pyrrole-2,4-diyl]carbonylimino[1-methyl-1H-pyrrole-2,4-diyl]carbonylimino]]bis- (9CI) (CA INDEX NAME)

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L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

- sозн

RN 149621-84-1 HCAPLUS
CN 1,3,5-Naphthalenetrisulfonic acid, 7,7'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino]bis- (9CI) (CA INDEX NAME)

RN 149621-85-2 HCAPLUS
CN 1,3-Naphthalenedisulfonic acid, 7,7'-{carbonothioylbis{imino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino||bis- {9CI} (CA INDEX NAME)

LB ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

PAGE 1-B

(Continued)

RN 149621~87-4 HCAPLUS
CN D-Glucose, 2,2'-[carbonylbis[imino(1-methyl-1H-pyrrole-2,4diyl]carbonylimino(1-methyl-1H-pyrrole-2,4-diyl]carbonylimino)]bis(2-deoxy-,6,6'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 149621-86-3 HCAPLUS
CN D-Glucose, 2,2'-|carbonylbis|imino(1-methyl-1H-pyrrole-2,4diyl)carbonylimino(1-methyl-1H-pyrrole-2,4-diyl)carbonylimino|]bis{2-deoxy-,6,6'-bis(hydrogen sulfate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

L8 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L8 ANSWER 31 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 18 Sep 1993

AB Comparison of the DNA cleavage activity of man-designed bleomycins demonstrates that bleomycins are small enzymes comprised of the catalytic site and a binding site. The linker moiety is shown to be significant for DNA binding, and inversion of its stereochem. results in a dramatic decrease in the DNA-cleaving efficiency. It can be said that bleomycin possesses a switching device in the B-aminoalaninamide moiety to regulate the in vivo activity. One of the man-designed BLMs shows excellent cytotoxicity against Li210.

ACCESSION NUMBER: 1993:508375 HCAPLUS

DOCUMENT NUMBER: 1193:508375 HCAPLUS

TITLE: Man-designed bleomycins based on the anticancer mechanism of natural bleomycins: Significance of the binding sites as enzyme models, of the stereochemistry of the linker moiety, and of a switching device in the B-aminoalaninamide moiety

AUTHOR(S): Ohno, Masaji Milly Takwa Takwa Japan

N-aminoalaninamide molety
Ohno, Masaji
Fac. Pharm. Sci., Univ. Tokyo, Tokyo, Japan
Proceedings of the Robert A. Welch Foundation
Conference on Chemical Research (1991), 35(Chem.
Front. Med.), 119-34
CODEN: PRAWAC, ISSN: 0557-1588 CORPORATE SOURCE: SOURCE:

DOCUMENT TYPE: LANGUAGE:

149352-73-8

RL: RCT (Reactant); RACT (Reactant or reagent)

RL: RCT (Reactant); RACT (Reactant or reagent)
(deprotection of)

149352-73-8 HCAPLUS
Carbamic acid, [4-[[5-[[[5-[[[5-[[[3-[dimethylamino)propyl]amino]carbonyl]1-methyl-1H-pycrol-2-yl]amino]carbonyl]-1-methyl-1H-pycrol-2yl]amino[carbonyl]-1-methyl-1H-pycrol-2-yl]amino]-4-oxobutyl]-,
1,1-dimethylethyl ester (9C1) (CA INDEX NAME)

PAGE 1-B

149330-07-4P

149330-07-49
REL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with distamycin)
149330-07-4 HCAPLUS
H-Pyrrole-2-carboxamide, 5-[[[5-[(4-amino-1-oxobutyl)amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-N-[5-[[[3-(dimethylamino)propyl]amino]carbonyl

L8 ANSWER 32 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

Entered STN: 07 Aug 1993
AB Nonintercalating DNA minor-groove binders may effectively inhibit the supercoiling activity of DNA gyrase (I) by influencing the enzyme recognition and cleavage site on DNA. For I from Streptomyces noursel, a wide range of inhibitory potency for different classes of ligands was observed This could be explained by a number of structural and binding factors of the ligands competing with I on the target site of DNA, the mechanism of which is different from the classical I inhibitors.

ACCESSION NUMBER: 1993:443973 HCAPLUS

DOCUMENT NUMBER: 1914:43973

Minor-groove binders are inhibitors of the catalytic

DOCUMENT NUMBER: TITLE: 119:43973
Minor-groove binders are inhibitors of the catalytic activity of DNA gyrases
Stoerl, K.; Stoerl, J.; Zimmer, Ch.; Lown, J. W.
Dep. Mol. Biol., Inst. Mol. Biol., Univ. Jena, Jena,
Germany
FEBS Letters (1993), 317(1-2), 157-62
CODEN: FEBLAL; ISSN: 0014-5793
JOURNAL

AUTHOR(S): CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE: Journal

JOURNAL TIPE: English

IT 148504-19-2 148504-20-5 148504-21-6

RL: BIOL (Biological study)

(DNA gyrase of Streptomyces noursei inhibition by, mechanism of)

RN 148504-19-2 HcAPPLUS

CN Heptanediamide, N.N'-bis[5-[[[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]- (9CI) (CA

PAGE 1-B

148504-20-5 HCAPLUS
Octanediamide, N,N'-bis[5-[[[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

ANSWER 31 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1-1-methyl-1H-pyrrol-2-yl)-1-methyl- (9CI) (CA INDEX NAME)

PAGE 1-B

- (CH2) 3 - NH2

PAGE 1-B

148504-21-6 HCAPLUS
Decanediamide, N,N'-bis[5-[[5-[[3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

L8 ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ENTERED Entered STN: 04 Oct 1992

AB HX1ZX2ZX3ZCONHCHZCHZC(:NH)NH2 (X1, X2, X3 = CONH or NHCO the case wherein

X1 = X2 = X3 = CONH being excluded; Z = 1-methyl-2, 4-pyrrolylene

throughout) were prepared as antiviral and antitumor agents (no data).

Thus, NOZCZCOZME and CONZCON3 (preparation each given) were heated with Et3N

and the product converted in 3 steps to OZNZHGOZCONHCHZCHZC(:NH)NH2 which

was hydrogenated and the product condensed with HCONHZCOZH (preparation given)

to give HCONHZCONHZNHCOZCONHCHZC(:NH)NH2.

ACCESSION NUMBER: 1992:330993 HCAPLUS

DOCUMENT NUMBER: 1992:330993 HCAPLUS

Preparation of distamycin analogs as antiviral

117:130993
Preparation of distamycin analogs as antiviral antitumor agents
Animati, Pabio: Arcamone, Federico; Lombardi, Paolo; Rossi, Cristina
Menarini, A., Industrie Farmaceutiche Riunite S.r.l., Italy, Bristol-Hyers Squibb S.p.A.
PCT Int. Appl., 39 pp.
CODEN: PIXXD2
Patent
English
1 INVENTOR (S):

PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 9209574	A2 19920611	WO 1991-EP2220	19911120
WO 9209574	A3 19920806		
W: AU, BB, BG,	BR, CA, CS, FI, F	HU, JP, KP, KR, LK, MC,	MG, MN, MW,
NO, PL, RO,	SD, SU, US		
RW: AT, BE, BF,	BJ, CF, CG, CH, C	CI, CM, DE, DK, ES, FR,	GA, GB, GN,
GR, IT, LU,	ML, MR, NL, SE, S	SN, TD, TG	
AU 9189178	A1 19920625	AU 1991-89178	19911120
PRIORITY APPLN. INFO.:		IT 1990-22154 A	19901122
		WO 1991-EP2220 A	19911120
OTHER SOURCE(S):	MARPAT 117:130993	3	

143158-63-8P 143158-64-9P 143158-65-0P 143363-83-1P

143303-83-19
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, in preparation of antiviral and antitumor

is)
143158-63-8 HCAPLUS
1H-Pyrrole-2-carboxylic acid, l-methyl-4-[[(1-methyl-4-nitro-1H-pyrrol-2yl)amino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

(Continued) ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

143158-59-2 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N4-[4-[[[4-{aminocarbonyl}-1-methyl-1H-pyrrol-2-yl]-n2-(3-amino-3-iminopropyl)-1-methyl- (9CI) (CA INDEX NAME)

143158-60-5 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-[5-[{(3-amino-3-iminopcopy)|amino|carbonyl}-1-methyl-1H-pyrrol-3-yl]-N4-[4-(formylamino)-1-methyl-1H-pyrrol-2-yl]-1-methyl- {9CI} (CA INDEX NAME)

ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1H-Pytrole-2-carboxylic acid, 1-methyl-4-[[(1-methyl-4-nitro-1H-pytrol-2-yllamino]carbonyll- (9CI) (CA INDEX NAME)

143158-65-0 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-(2-cyanoethyl)-1-methyl-N4-(1-methyl-4-ntro-1H-pyrrol-2-yl)- (9CI) (CA INDEX NAME)

143363-83-1 HCAPLUS
1H-Pyrrole-2,4-dicarboxamide, N2-(3-amino-3-iminopropyl)-1-methyl-N4-(1-methyl-4-nitro-1H-pyrrol-2-yl)-, monohydrochloride (9CI) (CA INDEX NAME) RN CN

ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

143158-61-6 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N4-[4-(aminocarbonyl)-1-methyl-1H-pyrrol-2yl]-N2-[5-[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3yl]-1-methyl- (9C1) (CA INDEX NAME)

143158-66-1 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N2-(3-amino-3-iminopropyl)-N4-[4-[[4-(formylamino)-1-methyl-1H-pyrrol-2-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-(9CI) (CA INDEX NAME)

ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

143158-67-2 HCAPLUS
1H-Pyrrole-2, 4-dicarboxamide, N4-[4-{[[4-{aminocarbonyl}]-1-methyl-1H-pyrrol-2-yl}amino]-carbonyl]-1-methyl-1H-pyrrol-2-yl}-N2-(3-amino-3-iminopropyl)-1-methyl- (9CI) (CA INDEX NAME)

ANSWER 35 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 17 Apr 1992

AB Title compds. [I; A = (un) substituted N-containing heterocyclylenediyl; Q = BN-RBR9R10, heterocyclyl, heterocyclylalkyl; B = alkylene alkylidene; R1 = H, Mer; R2 = H, alkyl; NQR2 = heterocyclyl group Q1; R3 = H, neg. charge; R6 = (un) substituted alkyl; R7-R10 = alkenyl, alkynyl, (un) substituted alkyl; m, n = 0-2) were prepared Thus, (2S, 4S)-4-(4-methoxybenzylthio)-2-pyrrolidinecarboxylic acid was N-protected and the product amidated with N-methylpiperazine to give, after hydrolysis, (2S, 4S)-4-mercapto-2-(4-methyl-1-piperaziny)carbonyl)-1-(4-hitrobenzyloxycarbonyl)pyrrolidine. The latter was stirred 5 h at .apprx.0° with 4-nitrobenzyl [Q1R, SR, 6S)-6-[(1R)-hydroxymethyl]-1-methyl-2-oxo-1-methyl-2-oxo-1-carbapenem-3-carboxylate which had been treated with Ph2P(0)C1 and the product treated with FSQOMe followed by catalytic hydrogenolysis to give title compound (1R, SS, 6S)-II which had MIC of SO.01 (no units given) against Staphylococcus aureus 209P and Escherichia coli NIHJ. I are resistant to dehydropeptidase I and B-lactamase.

ACCESSION NUMBER: 1992:151432 KCAPLUS

DOCUMENY NUMBER: 1992:151432 KCAPLUS

Carbapenems and analogs as antibiotics

116:151432
Preparation of { (piperaziniocarbonyl) pyrrolidinylthio} carbapenems and analogs as antibiotics
Kawamoto, Isao: Miyauchi, Masao: Nakayama, Eiji; Endo, Rokuro: Ohya, Satoshi: Utaui, Yukio
Sankyo Co., Ltd., Japan
Eur. Pat. Appl, 117 pp.
CODEN: EPXXDW
Patent INVENTOR (S):

PATENT ASSIGNEE (S):

SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	TENT NO		KI	ND DATE	APE	PLICATION NO.	DATE
EΡ	443883		A			1991-301497	19910225
	R: A1	r, BE,	CH, DE	, DK, ES,	FR, GB, GF	R. IT. LI. LU.	NL. SE
JP	0421108	3	А	2 1992	0803 JP	1991-27059	19910221
CA	2036941	Ł	А	A 1991	0824 CA	1991-2036941	19910222
FI	9100860)	А	1991	0824 FI	1991-860	19910222

Page 4830/08/2005

EN ANSWER 34 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

Entered STN: 23 Aug 1992

AB Various aliphatic N-acyl derivs, and an N-phthalidyl derivative of the model compound N-bensyloxycarbonyl-glycyl-L-prolineamide (2-Gly-ProNH2) were synthesized to assess their suitability as produm forms for the C-terminal prolineamide residue occurring in several peptides (e.g. TRH) with the aim of protecting the peptide against prolyl endopeptidase in the gut prior to absorption. Whereas Z-Gly-ProNH2 was rapidly hydrolyzed in a rabbit gut homogenate, used as a source of prolyl endopeptidase, the N-acyl derivs. were found to afford protection by a factor of 1.5-6. The stability of the N-acyl derivs. in the gut homogenate decreased with increasing chain length within the acyl group. The N-phthalidyl derivative, on the other hand, degraded even faster than the parent compound The derivs. were all converted quant. into the parent peptide in human plasma solns, via hydrolysis catalyzed by non-specific plasma esterases. The results suggest that by appropriate N-acylation it may be feasible to improve the stability of a C-terminal prolineamide moiety toward prolyl endopeptidase. The combination of increased stability in the intestine and higher lipophilicity of the N-acyl prodrugs might render it possible to improve the delivery characteristics of peptides containing a C-terminal prolineamide moiety.

ACCESSION NUMBER: 117:6326

FITTLE:

117:76326
Prodrugs of peptides. 17. Bioreversible derivatization of the C-terminal prolineamide residue in peptides to afford protection against prolyl endopeptidase Moess, Judi; Bundgaard, Hans Dep. Pharm. Chem., R. Dan. Sch. Pharm., Copenhagen, Den.

AUTHOR(S): CORPORATE SOURCE:

Den. International Journal of Pharmaceutics (1992), 82(1-2), 91-7 CODEN: IJPHDE; ISSN: 0378-5173 Journal SOURCE:

DOCUMENT TYPE: LANGUAGE:

142755-61-1P

142755-61-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and hydrolysis of, for protection against prolyl endopeptidase)
142755-61-1 HCAPLUS
L-Prolinamide, N-[(phenylmethoxy|carbonyl]glycyl-N-(1,3-dihydro-3-oxo-1isobenzofuranyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 AN:	WER 35	OF 41	HCAPLUS	COPYRIGHT	2005 /	ACS on	STN	(Cont	inued)
FI	96863		В	19960531					
FI	96863		c	19960910					
МО	9100723		A	19910826	NO	1991-	723		19910222
МО	178498		В	19960102					
NO	178498		С	19960410					
ΑU	9171322		A1	19910829	AU	1991-	71322		19910222
AU	646012		B2	19940203					
HU	58100		A2	19920128	HU	1991-	620		19910225
ZA	9101344		A	19921125	ZA	1991-	1344		19910225
CZ	289263		B6	20011212	cz	1991-	483		19910225
US	5310735		A	19940510	US	1992-	938483		19920831
RU	2059639		C1	19960510	RU	1993-	4744		19930315
us	5420119		A	19950530	US	1993-	143996		19931027
PRIORIT	APPLN.	INFO. :			JP	1990-	42796	A	19900223
					JP	1990-	212283	A	19900810
					US	1991-	658975	B1	19910221
					US	1992-	938483	A3	19920831
					US	1993-	60817	B1	19930512
	OURCE (5)		MARPAT	116:15143	32				

(Continued)

EN ANSWER 36 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 05 Oct 1991

AB Bifunctional mols., e.g. tri-, tetra-, penta-, and hexa-nmethylpyrrolecatboxamide-EDTA, bis(EDTA-distanycin), etc., are prepared by
reacting a DNA intercalator (p-carboxymethidium, etc.) or DNA groove
binder (netropsin, distanycin, etc.) with 1,3-diaminopropane followed by
condensation with EDTA. These mols. are used for cleaving single- or
double-stranded DNA in the presence of Fe(II) and O with sequence
specificity which is either similar to or not available with naturally
occurring restriction enzymes. Thus, bis(EDTA-distanycin)phenoxazone was
prepared by using 3-benzyloxy-4-methyl-2-nitrobenzoic acid and
4-nitro-tri-N-methylpyrrole-2-carboxylic acid as starting materials, and
showed 100% cleavage of plasmid pBR322 DNA at ≥0.1 μM in the
presence of Fe(II), O, and dithiothretiol.

ACCESSION NUMBER: 115:131393 HCAPLUS
DOCUMENT NUMBER: 115:131393

TITLE: Preparation of bifunctional molecules having a DNA
intercalator or DNA groove binder linked to EDTA for
cleaving double-stranded DNA
Dervan, Petch B., Hertzberg, Robert P.
California Institute of Technology, USA
SUS-CS-SPD, Cont.-1n-part of U.S. 4,665,184.

DOCUMENT TYPE: Patent
LANGUAGE: English

DOCUMENT TYPE: LANGUAGE: LANGUAGE: Patent English FAMILY ACC. NUM. COUNT: 2 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4942227	A	19900717	US 1987-6442	19870123
US 4665184	A	19870512	US 1986-860604	19860507
PRIORITY APPLN. INFO.:			US 1982-338327 B2	19820111
			US 1983-540914 B1	19831012
			US 1986-860604 AZ	19860507
			US 1982-338332 A2	19820111
OTHER SOURCE(S):	MARPAT	115:131393		
IT 134986-15-5P				

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and reaction of, in preparation of bifunctional mols. having a

intercalator or DNA groove binder linked to EDTA for specific DNA

ANSWER 37 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 08 Dec 1990

AB Title compds. I [R2 = H, alkyl, Cl, (un)substituted Ph, (un)substituted Ph(PhH2; R4 = N, 1 or 2 substituents such as alkyl, HO, alkoxy, halo in 4-, 5-, 6-, or 7 position; alk = (un)substituted o, =alkylene (CH2)n; n = 2-6; NB = N3, H2N, alkylamino, hydroxyalkylamino, morpholino, thiomorpholino, piperidino, pyretidino, alkylamino, providino, aretidino, pyrrolidino, aretidino, are prepared II [R = R3CZ, R3COCH:CH, R3CO; R3 = cyclohexyl, heterocycylphenyl, cun)substituted and pyrolidino, aretidino, and byrolidino, aretidino, and antirheumatic activities. II [R = 3-(OX)C6H4CO; R1 = NBANL, BNCHZCH(OH)CH2] were also prepared and found to possess analgesic, antiinflammatory and antirheumatic activities. II [R = 3-(OX)C6H4CO; R1 = 2-morpholinoethyl; R2 = Me; R4 = H] in EtOAc and AcOH was reduced with H over Pt oxide to give 831 II [R = 3-(HZN)C6H4CO; R4 = morphoninoethyl; R2 = Me; R4 = H] in EtOAc and AcOH was reduced with H over Pt oxide to give 831 II [R = 3-(HZN)C6H4CO; R4 = morphoninoethyl; R2 = Me; R4 = H] (III). III, on oral administration, showed and EDOS in acetylcholine-induced abdominal constriction and antibradykinin test of 16 and 53 mg, resp., and on the rat paw flexion test 0.12i at 100 mg/kg.

ACCESSION NUMBER: 1990:611828 HCAPLUS

DOCUMENT NUMBER: 1990:611828 HCAPLUS

INVENTOR(S): Bell, Malcolm R.

PREPATENT ASSIGNEE(S): Sterling Drug Inc., USA

CODE: CAXXA4

DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent

LANGUAGE: English

DOCUMENT TYPE: LANGUAGE: Patent FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 1258070	A2	19890801	CA 1988-576124	19880830
US 4581354	A	19860408	US 1985-755239	19850715
CA 1246563	Al	19881213	CA 1985-488073	19850802
US 4634776	A	19870106	US 1985-810942	19851219
US 32761	E	19881004	US 1987-29302	19870323
CA 1255305	A2	19890606	CA 1988-576122	19880830
CA 1255316	A2	19890606	CA 1988-576123	19880830
CA 1255312	A2	19890606	CA 1988-576125	19880830
CA 1258069	A2	19890801	CA 1988-576121	19880830
US 4885295	A	19891205	US 1988-255305	19881011
FI 8903253	A	19890704	FI 1989-3253	19890704
FI 8903254	A	19890704	FI 1989-3254	19890704
FI 8903255	A	19890704	FI 1989-3255	19890704
FI 8903256	A	19890704	FI 1989-3256	19890704
FI 8903257	A	19890704	FI 1989-3257	19890704
US 4978664	A	19901218	US 1989-409913	19890920
NO 9003304	A	19860207	NO 1990-3304	19900725

Page 4930/08/2005

	NO 9003305	A	19860207	NO	1990-3305		19900725		
	NO 9003306	Â	19860207		1990-3306		19900725		
	US 5013732	A	19910507	US	1990-559787		19900730		
PRIC	RITY APPLN. INFO.:			US	1984-637931	А	19840806		
				US	1985-755239	А	19850715		
				CA	1985-488073	A3	19850802		
				FI	1985-2973	A	19850801		
				NO	1985-3066	A1	19850802		
				US	1985-810942	A3	19851219		
				US	1986-928335	A1	19861107		
				US	1988-255305	A3	19881011		
				US	1989-409913	A3	19890920		
OTHE	R SOURCE(S):	CASRE	ACT 113:2118	28;	MARPAT 113:21182	8			
IT	125019-12-7P								
	RL: BAC (Biologica	l activ	ity or effec	tor.	except adverse)	: BS	U (Biological		
	study, unclassifie								
						nera	peucic use,,		
	BIOL (Biological a								
	(preparation of	, as an	algesic, ant	iint	lammatory, and a	ntir	heumatic)		
RN	125019-12-7 HCAPI								
CN	1H-Indole-3-carboxamide, N-methyl-1-(1-methyl-2-(4-morpholinyl)ethyl)-N-1H-								
	DUTES 1-2-41- mone	hudroch	laride (OCT)	"	A THIRDY HAMPI	-	• •		

(Continued)

L8 ANSWER 37 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 21 Jan 1989 GI

AB The title compds. [I, Rl, R2 = H, Cl-6 alkyl, C3-7 cycloalkyl,
 (un)substituted heterocyclyl; X = H, Cl-4 alkyl, Cl-4 alkoxy, Cl-4
 alkylthio, Br, Cl, F; Y = X, C3-6 cycloalkyl, CF3, NO2, MeCO, EtCO, PtCO,
 PhCO, thenoyl; adjacent XY = OCH20) were prepared as inflammation inhibitors
 and analgesics (no data). To a slurry of 13.3 g oxindole (2-indolinone)
 in PhMe was added 15.6 g ClSO2NCO and the mixture heated on a steam bath to
 give 1-{chlorosulfonyl}carbamoyl]oxindole which was heated in aqueous HOAc to
 give 11.48 g 1-carbamoyloxindole. The latter (1.0 g) and 1.28 g
 2,4-C12C6H3NCO were stirred at 1 h 0-5* in DMF containing bt3N,
 followed by addition of in HCL and stirring 20 min. to give 290 mg I (R1 =
 2.4-C12C6H3N.Z = X = Y = H).

ACCESSION NUMBER: 1989:23728 HCAPLUS

DOCUMENT NUMBER: 1989:23728 HCAPLUS

INVENTOR(S): Kadin, Saul B.

Preparation of oxindole-1,3-dicarboxamides as
 antiinflammatory agents

Kadin, Saul B.

PSTATENT ASSIGNEE(S): Pfizer Inc., USA

U.S., 30 pp. Cont.-in-part of U.S. Ser. No. 753,200,
 abandoned.

CODEN: USXXAM

POCUMENT TYPE:

LANGUAGE: WING CODEN:

DOCUMENT TYPE: LANGUAGE: LANGUAGE: FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 4725616	A	19880216	US 1987-8105		19870120
ZA 8605019	A	19880224	ZA 1986-5019		19860707
DD 251971	A5	19871202	DD 1986-292280		19860708
US 4791129	A	19881213	US 1987-118123		19871109
PRIORITY APPLN. INFO.:			US 1985-753200	A2	19850709
			US 1987-8105	A3	19870120

OTHER SOURCE(S): CASREACT 110:23728: MARPAT 110:23728 IT 107315-25-3P 107315-36-6P 107315-56-0P 107315-80-0P

107315-80-0P
RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiinflammatory)
107315-25-3 HCAPLUS
1H-Indole-1,3-dicarboxamide, 2,3-dihydro-2-oxo-N3-2-thienyl- (9CI) (CA INDEX NAME)

ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

107315-36-6 HCAPLUS
1N-Indole-1,3-dicarboxamide, 5-chloro-2,3-dihydro-2-oxo-N3-2-thienyl(9C1) (CA INDEX NAME)

107315-56-0 RCAPLUS
1H-Indole-1,3-dicarboxamide, 2,3-dihydro-N1-(4-methoxyphenyl)-2-oxo-N3-2-thienyl- (9C1) (CA INDEX NAME)

107315-80-0 HCAPLUS

5H-1,3-Dioxolo(4,5-f)indole-5,7-digarboxamide, 6,7-dihydro-N5-(4-methoxyphenyl)-6-oxo-N7-2-thienyl- (9CI) (CA INDEX NAME)

ANSWER 39 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 15 May 1987

AB The title compds. [I: n = 0-4; R = NHR3 [R3 = CON(NO)R4 [R4 = C1-4 (halo)alkyl], CO(CH2)mR5 (R5 = halo, oxiranyl, methyloxiranyl, aziridinyl, cyclopropyl, moiety of alicyclic α,β-unsatd. ketone or lactone: m = 0-41), NR6R7 [R6, R7 = oxiranylmethyl, aziridinylmethyl, substituted C2-4 alkyl: l of R6, R7 = H, the other as abovel, NO2, NH2, NNCHO: R1 = H, C1-6 alkyl: R2 = substituted C1-6 alkyl] and their pharmaceutically tolerable salts, useful as antiviral and antineoplastic agents, were prepared by 6 methods, e.g. reaction of amthopyrrolecatoxamide II (q = 1-5) with nitropyrrole III (Z = leaving group) to give I (R = NO2).
3-[1-Methyl-4-1-[1-methyl-4-d-amtnpyrrole-2-carbonaldo]pyrrole-2-carboxamido]pyrole-2-carboxamido]pyrole-2-

106:156157
Poly-4-aminopyrrole-2-carboxamide derivatives, procedure for their preparation, and antiviral and antineoplastic pharmaceuticals containing them Arcamone, Federico; Mongelli, Nicola; Penco, Sergio Farmitalia Carlo Etba S.p.A., Italy Ger. Offen., 35 pp.
CODEN: GWXXEX
Patent German INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3623880	A1	19870129	DE 1986-3623880	19860715
US 4766142	A	19880823	US 1985-783588	19851003
SE 8603098	А	19870117	SE 1986-3098	19860711
SE 468642	В	19930222		
SE 468642	c	19930617		

L8	ANSWER 39 OF 41	HCAPLUS	COPYRIGHT	2005 ACS on STN	(Continued)
	AT 8601888	A	19880415	AT 1986-1888	19860711
	AT 387013	В	19881125		
	AU 8660202	Al	19870122	AU 1986-60202	19860714
	AU 587841	B2	19890831		
	NL 8601837	А	19870216	NL 1986-1837	19860714
	HU 43088	A2	19870928	HU 1986-2904	19860714
	HU 205949	В	19920728		
	ES 2000502	A6	19880301	ES 1986-290	19860714
	IL 79402	Al	19910610	IL 1986-79402	19860714
	BE 905110	Al	19870115	BE 1986-216924	19860715
	DK 8603359	А	19870117	DK 1986-3359	19860715
	NO 8602860	A	19870119	NO 1986-2860	19860715
	NO 168826	В	19911230		
	NO 168826	С	19920408		
	FR 2585018	A1	19870123	FR 1986-10294	19860715
	FR 2585018	Bl	19890713		
	ZA 8605263	А	19870325	ZA 1986-5263	19860715
	JP 62077362	A2	19870409	JP 1986-164879	19860715
	SU 1544185	A3	19900215	SU 1986-4027809	19860715
	CH 674206	А	19900515	CH 1986-2820	19860715
	CA 1285934	Al	19910709	CA 1986-513760	19860715
	FI 8602959	A	19870117	FI 1986-2959	19860716
	FI 83640	В	19910430		
	FI 83640	С	19910812		
	GB 2178036	A1	19870204	GB 1986-17292	19860716
	GB 2178036	B2	19890816		
	CN 86104787	А	19870218	CN 1986~104787	19860716
	CN 1018825	В	19921028		
	CS 276981	B6	19921118	CS 1986-5412	19860716
	SU 1609445	A3	19901123	SU 1987-4203699	
PRIC	RITY APPLN. INFO.	:		GB 1985-17922	A 19850716
				GB 1986-13594	A 19860604
IT	107580-36-9P				

107580-36-99
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of, as antiviral and antineoplastic agent)
107580-36-9 HCAPLUS
1H-Pyrrole-2-carboxamide, N-[5-[[[5-[[3-(dimethylamino)propyl]amino]carbo
nyl]-1-methyl-1H-pyrrol-3-yllamino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1methyl-4-[([1-methyl-4-[[(1-methyl-4-filtro-1H-pyrrol-2-yl)amino]carbonyl]1H-pyrrol-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 01 May 1987

AB The title compds. I [X = H, Br, Cl, F, Cl-4 alkyl, alkylthio, alkoxy, C3-6 cycloalkyl, No2, CF3, C2-4 acyl, Bz, thenoyl: Y = H, Br, Cl, Cl-4 alkyl, alkoxy, alkylthio; optionally XY = 4,5-, 5,6-, 6,7-OCH2O: A = NNR2, R3, NHCOR3; R1, R2 = H, Cl-6 alkyl, C3-7 cycloalkyl, heterocyclyl, (substituted)Ph; R3 = Cl-6 alkyl, Ph] and their salts, prepared by the reaction of the appropriate oxindole with R1NCO or R1NNI2, are useful as antinfilammatory and analgesic agents (no data). To 1-carbamoyloxindole, and E1N in DNF, was added 2,4-C12C6H3NCO to give after addition of 1N HCl I (X = Y = H; A = NH2; R1 = 2.4-C12C6H3).

ACCESSION NUMBER: 1987:138254 HCAPLUS
DOCUMENT NUMBER: 1987:138254 HCAPLUS
DOCUMENT NUMBER: 1987:138254 HCAPLUS
INVENTOR(S): 25 as antinflammatory and analgesic agents
XAII, Saul Bernard
Frier Inc., USA
EUR. Pat. Appl., 56 pp.
CODEN: EYKENDW
DOCUMENT TYPE: Patent Appl., 56 pp.
CODEN: EYKENDW
PATENT INFORMATION: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA	TENT NO.		KI	D	DATE	AP	PLICATION NO.		DATE
	208510		A.		19870114	EP	1986-305144		19860702
	208510		A:		19880302				
EP	208510		В:		19910911				
	R: AT,	BE,	CH, DE,	FR,	GB, IT,	LI, L	U, NL, SE		
บร	4678802		A		19870707	US	1986-825017		19860131
AT	67185		ε		19910915	AT	1986-305144		19860702
CA	1286663		A:		19910723	CA	1986-513184		19860707
DK	8603242		A		19870110	DK	1986-3242		19860708
FI	8602882		А		19870110	FI	1986-2882		19860708
NO	8602750		А		19870112	NO	1986-2750		19860708
JP	62026269		A2		19870204	JP	1986-160675		19860708
JP	06010193		B		19940209				
AU	8659847		A.		19870409	AU	1986-59847		19860708
AU	566065		B		19871008				
HU	41386		A.		19870428	HU	1986-2844		19860708
HU	198015		8		19890728				
ES	2001855		A	,	19880701	ES	1986-191		19860708
IL	79356		A1		19900319	IL	1986-79356		19860708
CN	86105309		A		19870114	CN	1986-105309		19860709
ES	2009227		A		19890916	ES	1987-3589		19871215
PRIORIT	Y APPLN.	INFO.	:			US	1985-753200	А	19850709
						US	1986-821296	A	19860122
							1986-825017		19860131
							1986-305144	A	

OTHER SOURCE(S): CASREACT 106:138254 IT 107315-25-3P 107315-36-6P 107315-56-0P

Page 5130/08/2005

LB ANSWER 39 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A NO2

ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)
107315-80-09
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as analgesic and antiinflammatory agent)
107315-25-3 HCAPLUS
HH-Indole-1,3-dicarboxamide, 2,3-dihydro-2-oxo-N3-2-thienyl- (9CI) (CA INDEX NAME)

107315-36-6 HCAPLUS 1H-Indole-1,3-dicarboxamide, 5-chloro-2,3-dihydro-2-oxo-N3-2-thienyl-(9CI) (CA INDEX NAME)

107315-56-0 HCAPLUS
1H-Indole-1,3-dicarboxamide, 2,3-dihydro-N1-(4-methoxyphenyl)-2-oxo-N3-2-thienyl-(9CI) (CA INDEX NAME)

107315-80-0 HCAPLUS
5H-1,3-Dioxolo[4,5-f]indole-5,7-dicarboxamide, 6,7-dihydro-N5-(4-

ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) methoxyphenyl)-6-oxo-N7-2-thienyl- (9CI) (CA INDEX NAME)

ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

77604-47-BP 77604-48-9P
RL: BRC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation); BIOL (Biological study): PREP (Preparation)
 (preparation and antiviral activity of)
77604-47-8 HCAPLUS
lH-Pyrrole-2-carboxamide, N-[5-[{(3-amino-3-iminopropyl)amino]carbonyl}-l-methyl-1H-pyrrol-2-yl)-l-methyl-15-[{(1-methyl-5-nitro-lH-pyrrol-2-yl)carbonyl]amino}-, monohydrochloride (9CI) (CA INDEX NAME)

77604-48-9 HCAPLUS
1H-Pyrrole-2-carboxamide, N-[5-[([3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl)-5-[[[5-(formylamino)-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

PAGE 1-B

77604-45-69
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and reduction-acylation reactions of) 77604-45-6 HCAPLUS

Page 5230/08/2005

ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 12 May 1984

AB Distamycin A and congocidine isomers and homologs I (R = NO2, HCONH) and II (R1 = NO2, H2NC(:NH)NHCH2CONH) were prepared and their cytotoxicity tested. Thus, acylation of H2NCH2CH2CN by 1-methyl-5-nitro-2-pyrrolecarbonyl chloride gave the pyrrolycarboxamidopropionitrile III, which was treated with EtOH-HCl at O' for 1 h and then with NH3(g) to give II (R1 = NO2). I were obtained by successive acylation-reduction reactions of 1-methyl-5-nitro-2-carboxylic acid. II (R1 = NO2) possessed the highest antiviral activity in the series, and was less toxic and had the same antiviral activity as distamycin and was less toxic and had the same antiviral activity as distamycin and was less toxic and had the same antiviral activity as distamycin and series.

ACCESSION NUMBER: 1981:192034 HCAPLUS

94:192034 HCAPLUS

111: R1: Preparation of distamycin and congocidine derivatives based on 2,5-dissubscituted byroles

125: HCAP

CORPORATE SOURCE:

Pharm. Sch., Hebrew Univ., Jerusalem, Israel Journal of Pharmaceutical Sciences (1980), 69(11), 1334-8

CODEN: JPMSAE; ISSN: 0022-3549

English

DOCUMENT TYPE: LANGUAGE: IT 77604-46-7P

77604-46-7P
RE: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(Preparation and aminolysis of, carboxamidemide derivative from)
77604-46-7 HCAPLUS
1H-Pyrrole-2-carboxamide, N-[5-[{(2-cyanoethyl)amino|carbonyl]-1-methyl-1H-pyrrol-2-yl)-1-methyl-5-{[(1-methyl-5-nitro-1H-pyrrol-2-yl)carbonyl]amino}(9CI) (CA INDEX NAME)

ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued) 1H-Pyrrole-Z-carboxamide, N-[5-[[(2-cyaneethyl)emino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-5-nitro-[9CI] (CA INDEX NAME)

77604-49-0P RL: SPN (Synthetic preparation); PREP (Preparation)

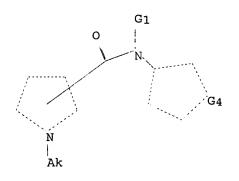
RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
77604-49-0 HCAPLUS
H-Pyrrole-2-carboxamide, 5-{{5-{{((aminoiminomethyl)amino)acetyl}amino}1-methyl-1H-pyrrol-2-yl]carbonyl]aminoj-N-[5-[{(3-amino-3iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]-1-methyl-,
dihydrochloride (9CI) (CA INDEX NAME)

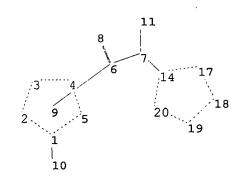
●2 HC1

PAGE 1-B

=> log y
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE
-29.93
-29.93

STN INTERNATIONAL LOGOFF AT 13:53:33 ON 30 AUG 2005





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

 $1-2 \quad 1-5 \quad 1-10 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-8 \quad 7-11 \quad 7-14 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

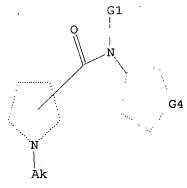
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 H, Me

G2 0, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

50 ANSWERS

=> s 11

SAMPLE SEARCH INITIATED 17:24:33 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 53526 TO 59914

PROJECTED ANSWERS: 10740 TO 13706

L2 50 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 17:24:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED 54653 ITERATIONS 11606 ANSWERS

SEARCH TIME: 00.00.04

L3 11606 SEA SSS FUL L1

=> fil hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

FULL ESTIMATED COST ENTRY SESSION 161.76 161.97

FILE 'HCAPLUS' ENTERED AT 17:24:59 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Page 430/08/2005

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 1844 L3

=> fil reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 2.45 164.42

FILE 'REGISTRY' ENTERED AT

FILE 'REGISTRY' ENTERED AT 17:25:13 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

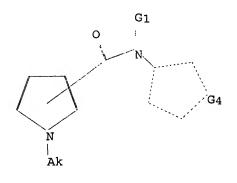
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

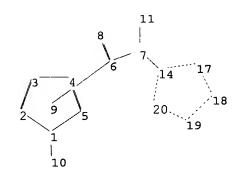
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\exp3update.str





chain nodes :
6 7 8 10 11
ring nodes :
1 2 3 4 5 14 17 18 19 20
chain bonds :
1-10 6-7 6-8 7-11 7-14
ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

 $1-2 \quad 1-5 \quad 1-10 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-8 \quad 7-11 \quad 7-14 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

G1:H,CH3

G2:0,S

G3:0,N

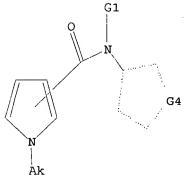
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L5 STRUCTURE UPLOADED

=> d 15 L5 HAS NO ANSWERS L5 STR



G1 H, Me

G2 O, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 17:26:27 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED

2000 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

53526 TO

59914

PROJECTED ANSWERS:

10553 TO

13495

50 SEA SSS SAM L5

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

=> s 15 full

FULL SEARCH INITIATED 17:26:34 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED

54653 ITERATIONS

11202 ANSWERS

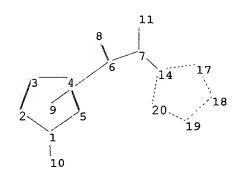
50 ANSWERS

SEARCH TIME: 00.00.07

L7

11202 SEA SSS FUL L5

Uploading C:\Program Files\Stnexp\Queries\ppp.str



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6 7 8 10 11
ring nodes :
1 2 3 4 5 14 17 18 19 20
chain bonds :
1-10 6-7 6-8 7-11 7-14
ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

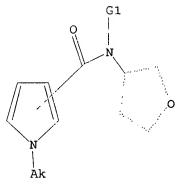
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L8 STRUCTURE UPLOADED

=> d 18 L8 HAS NO ANSWERS L8 STR



G1 H,Me

G2 O, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 18

SAMPLE SEARCH INITIATED 17:28:03 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED

1636 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

30294 TO 35146

PROJECTED ANSWERS:

0 TO

Ь9

0 SEA SSS SAM L8

=> s 18 full

FULL SEARCH INITIATED 17:28:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 33735 TO ITERATE

100.0% PROCESSED 33735 ITERATIONS

6 ANSWERS

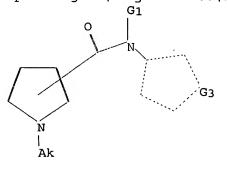
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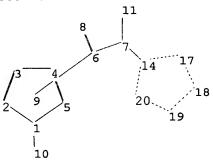
L10

6 SEA SSS FUL L8

=>

Uploading C:\Program Files\Stnexp\Queries\oooo.str





chain nodes : 6 7 8 10 11

ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

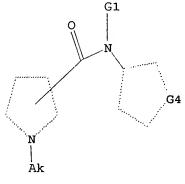
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L11 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me

G2 0,S

G3 O, N

G4 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l11

SAMPLE SEARCH INITIATED 17:29:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2664 TO ITERATE

Page 1030/08/2005

75.1% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 50185 TO 56375

PROJECTED ITERATIONS: 50
PROJECTED ANSWERS: 10

10244 TO 13144

50 ANSWERS

L12 50 SEA SSS SAM L11

=> fil hcaplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
325.67
490.09

FILE 'HCAPLUS' ENTERED AT 17:30:42 ON 30 AUG 2005
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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 110

L13 1 L10

=> d ed abs ibib hitstr 113

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 12 May 1984

H2CH (OR2) CH (CH2CHMe2) NHC (:X) CH (OR3) CH (OR4) CHR5CHR6COR7

CH (CH2CHMe2) NHC(:X) CH (OR3) CH (OH) CHR5CHR6COR7 II

AB Seven compds. with antiulcer activity, produced by Bacillus pumilus strain AI-77 during aerobic culture, have the structures I and II. These compds. also have antiinflammatory, anticholesteremic, antiarrhythmic, and vasodilatory activities and are intermediates for preparation of further compds. with these activities. For example, II-HCI (X = NM; R = R3 = R6 = H; R5 = NM2; R7 = OH) [77715-24-3] was produced by aerobic cultivation of B. pumilus AI-77 in 100 L defatted soybean meal-qlucose-salts medium for 20 h at 30', and was purified from the culture filtrate by chromatog, on Amberlite IRc-50 and XAD-2; the yield was 4.3 g. This compound at 50 mg/kg i.p. provided 100% protection against streas-induced ulcers in rats. The other 6 compds. were produced by B. pumilus in defatted soybean meal-corn steep liquor-sucrose-salts medium and separated by chromatog.

ACCESSION NUMBER: 1981:478461 HCAPLUS

1981:478461 HCAPLUS 95:78461 AI-77 compounds and their pharmaceutically acceptable TITLE:

PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan Neth. Appl., 221 pp. CODEN: NAXXAN

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE NL 8003985 NL 187069 NL 187069 JP 56012352 JP 63034863 19810113 NL 1980-3985 19800710 19910516 JP 1979-86892 19790711 JP 56158778 JP 02046585 JP 1980-61685 19800512

L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

77676-14-3 HCAPLUS
Hexonic acid, 2,3,6-trideoxy-6-[(1-{3,4-dihydro-8-hydroxy-1-oxo-1H-2-benzopyran-3-y1)-3-methylbutyl]amino]-3-[(1-methyl-1H-pyrrol-2-y1)carbonyl]amino]-6-oxo-, \(\gamma\)-lactone (9CI) (CA INDEX NAME)

77677-19-1 HCAPLUS
Hexonic acid, 3-{{|(1-acetyl-1H-pyrrol-2-yl)carbonyl}amino}-2,3,6-trideoxy-6-{|(1-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl)amino}-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

77677-24-8 HCAPLUS
Hexonic acid, 3-[[(1-acetyl-lH-indol-3-yl)carbonyl]amino]-2,3,6-trideoxy-6-[[(1-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

(Continued) 19800704 19800708 DE 1980-3026214 19800710 19800710 19800711 19870507 JP 1987-109723 JP 1979-86892 JP 1980-61685 PRIORITY APPLN. INFO.: A 19790711 A 19800512

T7676-02-9 T7676-13-2 T7676-14-3

T7677-19-1 T7677-2-8 T7677-2-8 T7676-14-3

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(ulcer-inhibiting activity of)

RN 77676-02-9 HCAPLUS

CN Hexonic acid, 3-[[(1-acety1-1H-indol-3-y1)carbony1]amino]-2, 3, 6-trideoxy-6
[[1-(3,4-dihydro-8-hydroxy-1-oxo-1H-2-benzopyran-3-y1)-3
methylbuty1]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

77676-13-2 HCAPLUS Hexonic acid, $3-[\{(1-acctyl-1H-pyrrol-2-yl)carbony]\}$ amino]-2,3,6-trideoxy-6-[$\{1-3,4-dihydro-8-hydroxy-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl]$ amino]-6-oxo-, γ -lactone (9CI) (CA INDEX NAME)

L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

77700-94-8 HCAPLUS
Hexonic acid, 2,3,6-trideoxy-6-[[1-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-y1)-3-methylbutyllamino]-3-[[(1-methyl-1H-pyrrol-2-y1)carbonyl]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

=> fil reg COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	9.84	499.93
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

FILE 'REGISTRY' ENTERED AT 17:31:41 ON 30 AUG 2005
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

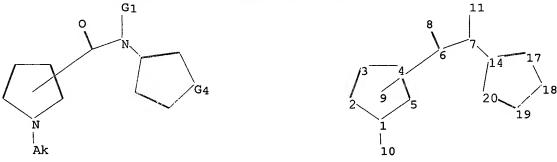
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\nnn.str



chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

 $1-2 \quad 1-5 \quad 1-10 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-8 \quad 7-11 \quad 7-14 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

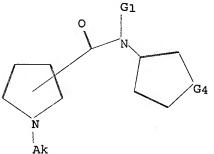
Match level :

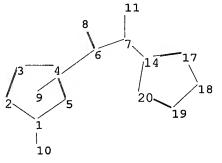
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L14 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\nnn.str





chain nodes :
6 7 8 10 11
ring nodes :
1 2 3 4 5 14 17 18 19 20
chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

Page 1430/08/2005

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L15 STRUCTURE UPLOADED

=> d 115 L15 HAS NO ANSWERS L15 STR

G1 H,Me

G2 O,S

G3 O,N

G4 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s 115

SAMPLE SEARCH INITIATED 17:33:09 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

53526 TO 59914

PROJECTED ANSWERS:

10420 TO 13344

L16

50 SEA SSS SAM L15

=> s l15 full

FULL SEARCH INITIATED 17:33:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED 54653 ITERATIONS

11063 ANSWERS

50 ANSWERS

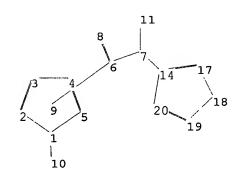
SEARCH TIME: 00.00.04

L17 11063 SEA SSS FUL L15

=>

Uploading C:\Program Files\Stnexp\Queries\yyyy.str

Page 1530/08/2005



chain nodes :
6 7 8 10 11
ring nodes :
1 2 3 4 5 14 17

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20 isolated ring systems :

containing 1 : 14 :

G1:H,CH3

G2:0,S

G3:0,N

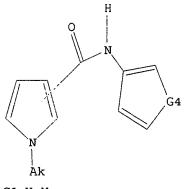
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L18 STRUCTURE UPLOADED

=> d 118 L18 HAS NO ANSWERS L18 STR



G1 H,Me

G2 0, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 118

SAMPLE SEARCH INITIATED 17:35:14 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1019 TO ITERATE

100.0% PROCESSED

1019 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

50 SEA SSS SAM L18

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

18465 TO 22295

PROJECTED ANSWERS:

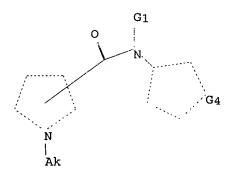
10098 TO 12980

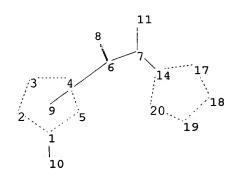
L19

=> log y COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 163.48 663.41

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -0.73

STN INTERNATIONAL LOGOFF AT 17:35:22 ON 30 AUG 2005





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

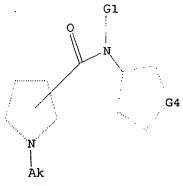
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G2 0,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 17:24:33 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

59914 53526 TO

PROJECTED ANSWERS: 10740 TO 13706

50 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 17:24:39 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED 54653 ITERATIONS 11606 ANSWERS

50 ANSWERS

SEARCH TIME: 00.00.04

11606 SEA SSS FUL L1 L3

=> fil hcaplus

SINCE FILE COST IN U.S. DOLLARS TOTAL

ENTRY SESSION FULL ESTIMATED COST 161.97 161.76

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 1844 L3

=> fil reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 2.45 164.42

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 17:25:13 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

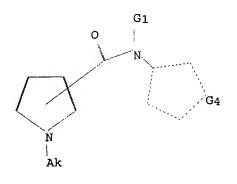
Please note that search-term pricing does apply when conducting SmartSELECT searches.

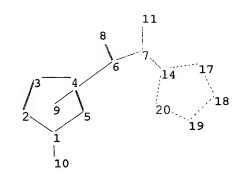
* The CA roles and document type information have been removed from * the IDE default display format and the ED field has been added, * effective March 20, 2005. A new display format, IDERL, is now * available and contains the CA role and document type information. * *

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\exp3update.str





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

 $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

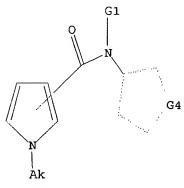
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G2 0, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 17:26:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED

2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

53526 TO 59914

PROJECTED ANSWERS:

10553 TO 13495

L6 50 SEA SSS SAM L5

=> s 15 full

FULL SEARCH INITIATED 17:26:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

100.0% PROCESSED 54653 ITERATIONS

11202 ANSWERS

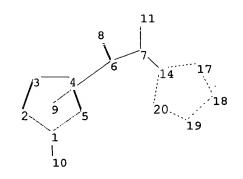
50 ANSWERS

SEARCH TIME: 00.00.07

L7 11202 SEA SSS FUL L5

=>

Uploading C:\Program Files\Stnexp\Queries\ppp.str



chain nodes : 6 7 8 10 11

ring nodes : 1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:0,N

G4:0,S,N

Match level :

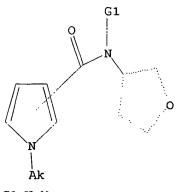
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS

STR



G2 O,S

G3 O,N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 18

SAMPLE SEARCH INITIATED 17:28:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED

1636 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

30294 TO 35146

PROJECTED ANSWERS:

0 TO

L9

0 SEA SSS SAM L8

=> s 18 full

FULL SEARCH INITIATED 17:28:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 33735 TO ITERATE

100.0% PROCESSED 337

33735 ITERATIONS

6 ANSWERS

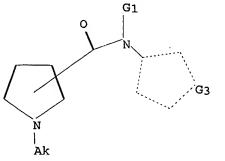
SEARCH TIME: 00.00.01

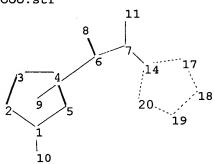
L10

6 SEA SSS FUL L8

=>

Uploading C:\Program Files\Stnexp\Queries\oooo.str





Page 930/08/2005

chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

 $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 14-17 \quad 14-20 \quad 17-18 \quad 18-19 \quad 19-20$

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H, CH3

G2:0,S

G3:0,N

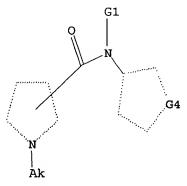
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L11 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me

G2 0, S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 111

SAMPLE SEARCH INITIATED 17:29:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2664 TO ITERATE

Page 1030/08/2005

75.1% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

50 ANSWERS

PROJECTED ITERATIONS: 50185 TO 56375 PROJECTED ANSWERS: 10244 TO 13144

L12 50 SEA SSS SAM L11

=> fil hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL FINTRY SESSION

FULL ESTIMATED COST ENTRY SESSION 325.67 490.09

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FILE COVERS 1907 - 30 Aug 2005 VOL 143 ISS 10 FILE LAST UPDATED: 29 Aug 2005 (20050829/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 110

L13 1 L10

=> d ed abs ibib hitstr 113

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 12 May 1984

H2CH (OR2) CH (CH2CHMe2) NHC (:X) CH (OR3) CH (OR4) CHR5CHR6COR7

CH (CH2CHMe2) NHC (:X) CH (OR3) CH (OH) CHR5CHR6COR7 II

AB Seven compds. with antiulcer activity, produced by Bacillus pumilus strain AI-77 during aerobic culture, have the structures I and II. These compds. also have antiinflammatory, anticholestermic, antiarchythmic, and vasodilatory activities and are intermediates for preparation of further compds. With these activities. For example, II-RG1 (X = NH; R = R3 = R6 = H; R5 = NH2; R7 = OH) [77715-24-3] was produced by aerobic cultivation of B. pumilus AI-77 in 100 L defatted sophean meal-glucose-salts medium for 20 h at 30°, and was purified from the culture filtrate by chromatog. on Amberlite IRc-50 and XAD-2; the yield was 4.3 g. This compound at 50 mg/kg i.p. provided 100% protection against stress-induced ulcers in rats. The other 6 compds. were produced by B. pumilus in defatted soybean meal-corn steep liquor-sucrose-salts medium and separated by chromatog.

ACCLESSION NUMBER: 1981:478461 HCAPLUS

DOUMPENT NUMBER: 95:78461

TITLE: AI-77 compounds and their pharmaceutically acceptable salts

1981:478461 HCAPLUS 95:78461 A1-77 compounds and their pharmaceutically acceptable salts Asahi Chemical Industry Co., Ltd., Japan Neth. Appl., 221 pp. CODEN: NAXXAN Patent

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 8003985	A	19810113	NL 1980-3985	19800710
NL '187069	В	19901217		
NL 187069	c	19910516		
JP 56012352	A2	19810206	JP 1979-86892	19790711
JP 63034863	B4	19880712		
JP 56158778	A2	19811207	JP 1980-61685	19800512
JP 02046585	84	19901016		

L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

77676-14-3 HCAPLUS Hexonic acid, 2,3,6-trideoxy-6-[[1-{3,4-dihydro-8-hydroxy-1-oxo-1H-2-benzopyran-3-y1}-3-methylbuty1]amino]-3-[[(1-methyl-1H-pyrrol-2-y1)carbony1]amino]-6-oxo-, γ -lactone (9CI) (CA INDEX NAME)

77677-19-1 HCAPLUS
Hexonic acid, 3-[{[1-acetyl-1H-pyrrol-2-yl)carbonyl]amino]-2,3,6-trideoxy-6-[[1-(6-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl]amino]-6-oxo-, \gamma-lactone (9CI) (CA INDEX NAME)

77677-24-8 HCAPLUS
Hexonic acid, 3-[([1-acetyl-1H-indol-3-yl)carbonyl]amino]-2,3,6-trideoxy-6[[1-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-yl)-3-methylbutyl]amino]6-oxo-, y-lactone (9CI) (CA INDEX NAME)

19800704 19800708 DE 1980-3026214 19800710 19800710 19870507 PRIORITY APPLN. INFO.: JP 1979-86892 JP 1980-61685 A 19790711 A 19800512

| OTHER SOURCE(S): CASREACT 95:78461 | T7676-02-9 77676-13-2 77676-14-3 | T7677-19-1 77677-29-1 77677-29-1 77677-29-1 77677-29-8 | RL: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): BIOL (Biological study) (ulcer-inhibiting activity of) | RN 77676-02-9 | HCAPLUS | RC: CASE | RC: CAS

//BVD-13-2 noteD03

Hexonic acid, 3-[[[1-acetyl-1H-pyrrol-2-yl]carbonyl]amino]-2,3,6-trideoxy-6-[[1-[3,4-dihydro-8-hydroxy-1-oxo-1H-2-benzopyran-3-yl]-3-methylburyl]amino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN (Continued)

77700-94-8 HCAPLUS
Hexonic acid, 2,3,6-trideoxy-6-[[1-(8-ethoxy-3,4-dihydro-1-oxo-1H-2-benzopyran-3-y1)-3-methylbutyllamino]-3-[[(1-methyl-1H-pyrrol-2-y1)carbonyllamino]-6-oxo-, y-lactone (9CI) (CA INDEX NAME)

=> fil reg COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	9.84	499.93
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

FILE 'REGISTRY' ENTERED AT 17:31:41 ON 30 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3 DICTIONARY FILE UPDATES: 29 AUG 2005 HIGHEST RN 862072-85-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

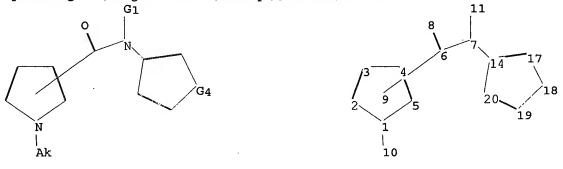
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> Uploading C:\Program Files\Stnexp\Queries\nnn.str



chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H, CH3

G2:0,S

G3:0, N

G4:0,S,N

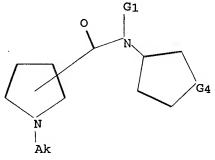
Match level:

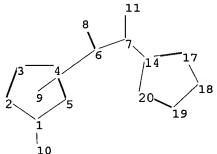
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L14 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\nnn.str





chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

G1:H,CH3

G2:0,S

G3:O,N

G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L15 STRUCTURE UPLOADED

=> d 115 L15 HAS NO ANSWERS L15 STR

G1 H,Me

G2 0,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

50 ANSWERS

=> s 115

SAMPLE SEARCH INITIATED 17:33:09 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2836 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 53526 TO 59914
PROJECTED ANSWERS: 10420 TO 13344

L16 50 SEA SSS SAM L15

=> s 115 full

FULL SEARCH INITIATED 17:33:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 54653 TO ITERATE

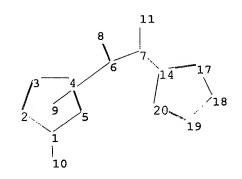
100.0% PROCESSED 54653 ITERATIONS 11063 ANSWERS

SEARCH TIME: 00.00.04

L17 11063 SEA SSS FUL L15

Uploading C:\Program Files\Stnexp\Queries\yyyy.str

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chain nodes : 6 7 8 10 11 ring nodes :

1 2 3 4 5 14 17 18 19 20

chain bonds :

1-10 6-7 6-8 7-11 7-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-17 14-20 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 4-5 6-7 6-8 7-11 7-14 14-17 14-20 17-18 18-19 19-20

isolated ring systems :

containing 1 : 14 :

G1:H,CH3

G2:0,S

G3:0,N

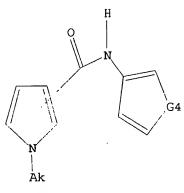
G4:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L18 STRUCTURE UPLOADED

=> d 118 L18 HAS NO ANSWERS L18 STR



G2 0,S

G3 O, N

G4 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> s 118

SAMPLE SEARCH INITIATED 17:35:14 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1019 TO ITERATE

100.0% PROCESSED

1019 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

22295

PROJECTED ITERATIONS:

18465 TO 10098 TO 12980

PROJECTED ANSWERS:

50 SEA SSS SAM L18

=> log y

L19

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	163.48	663.41
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.73

STN INTERNATIONAL LOGOFF AT 17:35:22 ON 30 AUG 2005